

FOR OFFICIAL USE ONLY

ACCESS DB # 181602  
PLEASE PRINT CLEARLY  
and 182836

Scientific and Technical Information Center

# SEARCH REQUEST FORM

Requester's Full Name: SABHA GHATA Examiner #: 74141 Date: 3/7/06  
Art Unit: 1616 Phone Number: 2-0622 Serial Number: 10/532847  
Location (Bldg/Room#): 4A45 (Mailbox #): 4270 Results Format Preferred (circle): PAPER DISK  
\*\*\*\*\*

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Cyclopropyl-Thienyl-Carboxamide

Inventors (please provide full names): Josef Ehrenfreund et al.

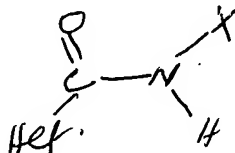
Earliest Priority Date: 371 of PCT/EP03/11805 10/24/03

## Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Cl 1-10



X = (X1), (X2) or (X3).

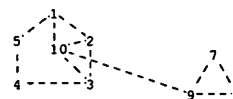
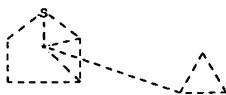
Het can be heterocyclic gp. Specific heterogps see cl 2.

Copy of claims enclosed

## STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: _____	____ NA Sequence (#)	____ STN      ____ Dialog
Searcher Phone #: _____	____ AA Sequence (#)	____ Questel/Orbit      ____ Lexis/Nexis
Searcher Location: _____	____ Structure (#)	____ Westlaw      ____ WWW/Internet
Date Searcher Picked Up: _____	____ Bibliographic	____ In-house sequence systems
Date Completed: _____	____ Litigation	____ Commercial      ____ Oligomer      ____ Score/Length
Searcher Prep & Review Time: _____	____ Fulltext	____ Interference      ____ SPDI      ____ Encode/Transl
Online Time: _____	____ Other	____ Other (specify)

**THIS PAGE BLANK (USPTO)**



ring nodes :

1 2 3 4 5 7 8 9

ring bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-9 8-9

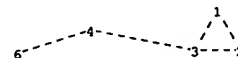
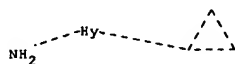
exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 7-8 7-9 8-9

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

**THIS PAGE BLANK (USPTO)**



chain nodes :

4 6

ring nodes :

1 2 3

chain bonds :

3-4 4-6

ring bonds :

1-2 1-3 2-3

exact/norm bonds :

1-2 1-3 2-3 3-4 4-6

Match level :

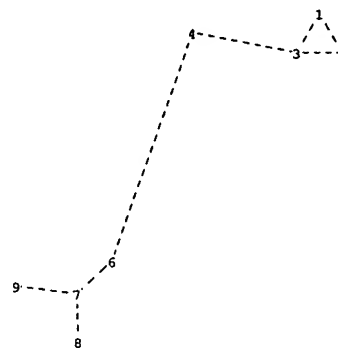
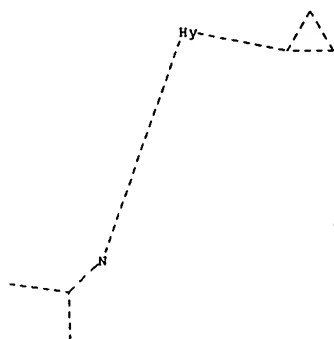
1:Atom 2:Atom 3:Atom 4:Atom 6:CLASS

Element Count :

Node 4: Limited

S,S1

**THIS PAGE BLANK (USPTO)**



chain nodes :

4 6

ring nodes :

1 2 3

ring/chain nodes :

7 8 9

chain bonds :

3-4 4-6 6-7

ring/chain bonds :

7-8 7-9

ring bonds :

1-2 1-3 2-3

exact/norm bonds :

1-2 1-3 2-3 3-4 4-6 6-7 7-8 7-9

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS

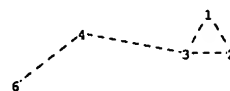
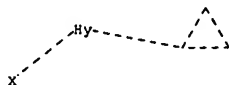
Element Count :

Node 4: Limited

S,S1

**THIS PAGE BLANK (USPTO)**





chain nodes :

4 6

ring nodes :

1 2 3

chain bonds :

3-4 4-6

ring bonds :

1-2 1-3 2-3

exact/norm bonds :

1-2 1-3 2-3 3-4 4-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 6:CLASS

Element Count :

Node 4: Limited

S,S1

**THIS PAGE BLANK (USPTO)**

# Search history - Part B

Qazi 10/532847

03/22/2006

=> d his full

(FILE 'HOME' ENTERED AT 09:22:18 ON 22 MAR 2006)

FILE 'REGISTRY' ENTERED AT 09:22:24 ON 22 MAR 2006

D SAV

ACT QAZ847STRA/A

-----

L1 STR

L2 ( 546562) SEA ABB=ON PLU=ON SC4/ES

L3 2304 SEA SUB=L2 SSS FUL L1

-----

ACT QAZ847STRB/A

-----

L4 STR

L5 ( 546562) SEA ABB=ON PLU=ON SC4/ES

L6 ( 2304) SEA SUB=L5 SSS FUL L4

L7 STR

L8 1135 SEA SUB=L6 SSS FUL L7

-----

ACT QAZ847STRC/A

-----

L9 STR

L10 ( 546562) SEA ABB=ON PLU=ON SC4/ES

L11 ( 2304) SEA SUB=L10 SSS FUL L9

L12 STR

L13 630 SEA SUB=L11 SSS FUL L12

-----

L14 STRUCTURE UPLOADED

L15 3 SEA SSS SAM L14

D SCA

L16 947626 SEA ABB=ON PLU=ON SC4/ESS

L17 2 SEA SUB=L16 SSS SAM L14

D SCA

L18 1954 SEA SUB=L16 SSS FUL L14

L19 1324 SEA ABB=ON PLU=ON L18 NOT L13

L20 1324 SEA ABB=ON PLU=ON L19 NOT L8

FILE 'CAPLUS' ENTERED AT 09:32:33 ON 22 MAR 2006

L21 222 SEA ABB=ON PLU=ON L20

L22 ANALYZE PLU=ON L21 1- RN : 20440 TERMS

D

FILE 'STNGUIDE' ENTERED AT 09:34:10 ON 22 MAR 2006

FILE 'REGISTRY' ENTERED AT 09:35:27 ON 22 MAR 2006

FILE 'STNGUIDE' ENTERED AT 09:38:23 ON 22 MAR 2006

FILE 'REGISTRY' ENTERED AT 09:56:04 ON 22 MAR 2006

FILE 'REGISTRY' ENTERED AT 09:56:19 ON 22 MAR 2006

SAVE TEMP L18 QAZ847STRD/A

L23 STRUCTURE UPLOADED

L24 3 SEA SUB=L18 SSS SAM L23

D SCA

L25 16 SEA SUB=L18 SSS FUL L23

SAVE TEMP QAZ847STRE/A L25

D SCA L25

FILE 'CAPLUS' ENTERED AT 09:58:56 ON 22 MAR 2006  
L26 14 SEA ABB=ON PLU=ON L25  
L27 10 SEA ABB=ON PLU=ON L25 (L) PREP/RL  
L28 90 SEA ABB=ON PLU=ON L18 (L) (RCT OR RGT OR RACT)/RL  
L29 9 SEA ABB=ON PLU=ON L27 AND L28

FILE 'CASREACT' ENTERED AT 10:01:42 ON 22 MAR 2006  
L30 3 SEA ABB=ON PLU=ON L25/PRO  
D SCA  
L31 33 SEA ABB=ON PLU=ON L18/RRT  
L32 1 SEA ABB=ON PLU=ON L31 (L) L30  
D SCA

FILE 'STNGUIDE' ENTERED AT 10:07:42 ON 22 MAR 2006  
D COST

FILE 'REGISTRY' ENTERED AT 10:19:16 ON 22 MAR 2006  
L33 STRUCTURE UPLOADED  
L34 0 SEA SUB=L18 SSS SAM L33  
L35 2 SEA SUB=L18 SSS FUL L33  
SAVE TEMP L35 QAZ847STRF/A

FILE 'CAPLUS' ENTERED AT 10:22:19 ON 22 MAR 2006  
L36 2 SEA ABB=ON PLU=ON L35  
D SCA

FILE 'REGISTRY' ENTERED AT 10:24:17 ON 22 MAR 2006  
L37 STRUCTURE UPLOADED  
L38 2 SEA SUB=L18 SSS SAM L37  
D SCA  
L39 72 SEA SUB=L18 SSS FUL L37  
SAVE TEMP QAZ847STRQ/A L39

FILE 'CAPLUS' ENTERED AT 10:25:52 ON 22 MAR 2006  
L40 29 SEA ABB=ON PLU=ON L39  
L\*\*\* DEL 29 S L39 AND L40  
L41 1 SEA ABB=ON PLU=ON L36 AND L40  
L42 12 SEA ABB=ON PLU=ON L39 (L) (RGT OR RCT OR RACT)/RL  
L43 2 SEA ABB=ON PLU=ON L35/PREP  
L44 1 SEA ABB=ON PLU=ON L42 AND L43

FILE 'STNGUIDE' ENTERED AT 10:29:46 ON 22 MAR 2006  
D COST

FILE 'CASREACT' ENTERED AT 10:34:00 ON 22 MAR 2006  
L45 0 SEA ABB=ON PLU=ON L35/PRO

FILE 'STNGUIDE' ENTERED AT 10:35:13 ON 22 MAR 2006

FILE 'REGISTRY' ENTERED AT 10:35:32 ON 22 MAR 2006  
D STAT QUE L18  
D STAT QUE L25  
D STAT QUE L35  
D STAT QUE L39

FILE 'CASREACT' ENTERED AT 10:37:48 ON 22 MAR 2006  
D QUE NOS L32

FILE 'CAPLUS' ENTERED AT 10:38:08 ON 22 MAR 2006  
D QUE NOS L26

L46                   D QUE NOS L27  
                      D QUE NOS L29  
                      14 SEA ABB=ON PLU=ON L26 OR L27 OR L29  
  
FILE 'CASREACT' ENTERED AT 10:40:36 ON 22 MAR 2006  
                      D IBIB ABS HIT L32 1  
  
FILE 'CAPLUS' ENTERED AT 10:40:37 ON 22 MAR 2006  
                      D IBIB ABS HITIND HITSTR L46 1-14  
  
FILE 'CASREACT' ENTERED AT 10:41:06 ON 22 MAR 2006  
                      D QUE NOS L45  
  
FILE 'CAPLUS' ENTERED AT 10:41:26 ON 22 MAR 2006  
                      D QUE NOS L36  
                      D QUE NOS L41  
                      D QUE NOS L43  
                      D QUE NOS L44  
L47                   2 SEA ABB=ON PLU=ON L36 OR L41 OR L43 OR L44  
                      D IBIB ABS HITIND HITSTR L47 1-2

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 MAR 2006 HIGHEST RN 877371-73-8

DICTIONARY FILE UPDATES: 20 MAR 2006 HIGHEST RN 877371-73-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE CAPLUS

Copyright of the articles to which records in this database refer is

held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Mar 2006 VOL 144 ISS 13  
FILE LAST UPDATED: 21 Mar 2006 (20060321/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

FILE STNGUIDE  
FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Mar 17, 2006 (20060317/UP).

FILE CASREACT  
Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 19 Mar 2006 VOL 144 ISS 12

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*      CASREACT now has more than 10 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Qazi 10/532847

03/22/2006

=&gt; file registry

FILE 'REGISTRY' ENTERED AT 10:35:32 ON 22 MAR 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2006 American Chemical Society (ACS)

STRUCTURE  
QUERIES

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 MAR 2006 HIGHEST RN 877371-73-8

DICTIONARY FILE UPDATES: 20 MAR 2006 HIGHEST RN 877371-73-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
```

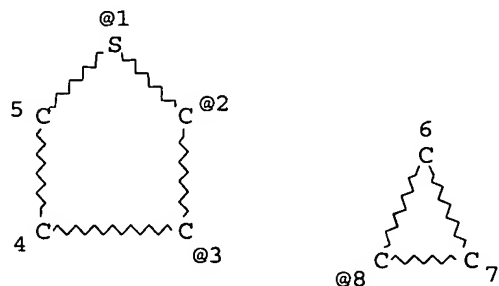
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=&gt; d stat que L18

L14 STR



VPA 8-1/2/3 U

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6

NSPEC IS R AT 7  
 NSPEC IS R AT 8  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

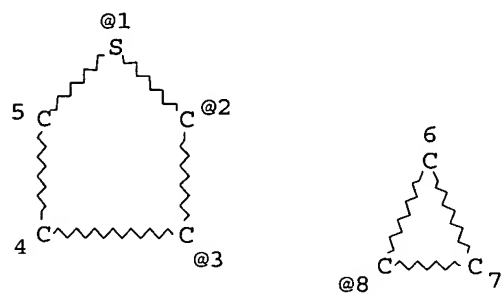
GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
 L16 947626 SEA FILE=REGISTRY ABB=ON PLU=ON SC4/ESS  
 L18 1954 SEA FILE=REGISTRY SUB=L16 SSS FUL L14

100.0% PROCESSED 894144 ITERATIONS  
 SEARCH TIME: 00.00.05

1954 ANSWERS

=> d stat que L25  
 L14 STR



VPA 8-1/2/3 U

NODE ATTRIBUTES:

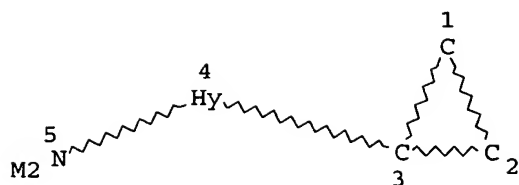
NSPEC IS R AT 1  
 NSPEC IS R AT 2  
 NSPEC IS R AT 3  
 NSPEC IS R AT 4  
 NSPEC IS R AT 5  
 NSPEC IS R AT 6  
 NSPEC IS R AT 7  
 NSPEC IS R AT 8

DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
 L16 947626 SEA FILE=REGISTRY ABB=ON PLU=ON SC4/ESS  
 L18 1954 SEA FILE=REGISTRY SUB=L16 SSS FUL L14  
 L23 STR





## NODE ATTRIBUTES:

```

HCOUNT  IS M2      AT  5
NSPEC     IS R       AT  1
NSPEC     IS R       AT  2
NSPEC     IS R       AT  3
NSPEC     IS C       AT  4
NSPEC     IS C       AT  5
DEFAULT MLEVEL IS ATOM
MLEVEL    IS CLASS  AT  5
DEFAULT ECLEVEL IS LIMITED
ECOUNT    IS M1 S    AT  4

```

## GRAPH ATTRIBUTES:

```

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

```

## STEREO ATTRIBUTES: NONE

```

L25      16 SEA FILE=REGISTRY SUB=L18 SSS FUL L23

```

```

100.0% PROCESSED      1600 ITERATIONS

```

```

16 ANSWERS

```

```

SEARCH TIME: 00.00.01

```

```

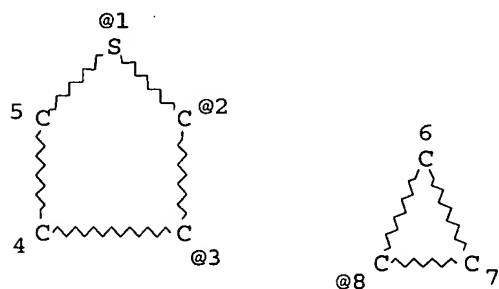
=> d stat que L35

```

```

L14      STR

```



```

VPA 8-1/2/3 U

```

## NODE ATTRIBUTES:

```

NSPEC     IS R       AT  1
NSPEC     IS R       AT  2
NSPEC     IS R       AT  3
NSPEC     IS R       AT  4
NSPEC     IS R       AT  5
NSPEC     IS R       AT  6
NSPEC     IS R       AT  7
NSPEC     IS R       AT  8
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

```

## GRAPH ATTRIBUTES:

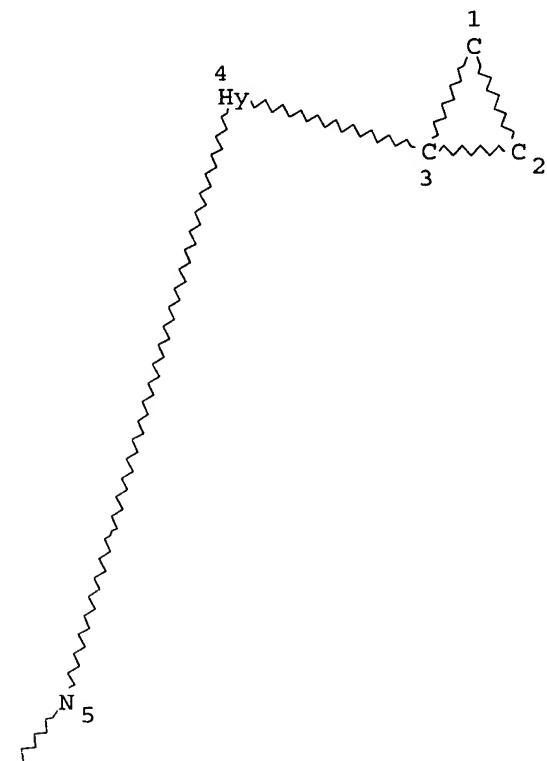
RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

## STEREO ATTRIBUTES: NONE

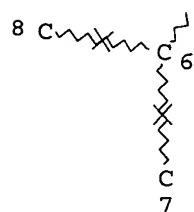
L16 947626 SEA FILE=REGISTRY ABB=ON PLU=ON SC4/ESS

L18 1954 SEA FILE=REGISTRY SUB=L16 SSS FUL L14

L33 STR



Page 1-A



Page 2-A

## NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS C	AT	4
NSPEC	IS C	AT	5
NSPEC	IS RC	AT	6
NSPEC	IS RC	AT	7
NSPEC	IS RC	AT	8

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 5 6 7 8  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M1 S AT 4

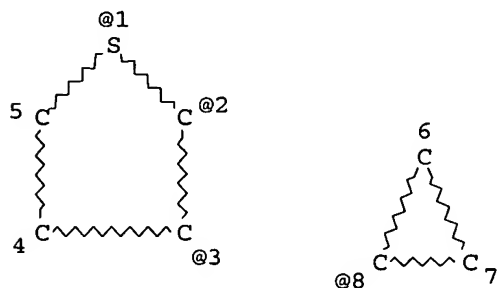
GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
 L35 2 SEA FILE=REGISTRY SUB=L18 SSS FUL L33

100.0% PROCESSED 1596 ITERATIONS  
 SEARCH TIME: 00.00.01

2 ANSWERS

=> d stat que L39  
 L14 STR



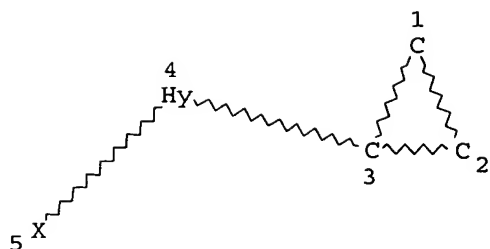
VPA 8-1/2/3 U  
 NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8

DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
 L16 947626 SEA FILE=REGISTRY ABB=ON PLU=ON SC4/ESS  
 L18 1954 SEA FILE=REGISTRY SUB=L16 SSS FUL L14  
 L37 STR



## NODE ATTRIBUTES:

```

NSPEC   IS R      AT    1
NSPEC   IS R      AT    2
NSPEC   IS R      AT    3
NSPEC   IS C      AT    4
NSPEC   IS C      AT    5
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS AT    5
DEFAULT ECLEVEL IS LIMITED
ECOUNT   IS M1 S   AT    4

```

## GRAPH ATTRIBUTES:

```

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS    5

```

## STEREO ATTRIBUTES: NONE

```

L39          72 SEA FILE=REGISTRY SUB=L18 SSS FUL L37

```

```

100.0% PROCESSED      1954 ITERATIONS
SEARCH TIME: 00.00.01

```

72 ANSWERS

=&gt; file casreact

```

FILE 'CASREACT' ENTERED AT 10:37:48 ON 22 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

```

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 19 Mar 2006 VOL 144 ISS 12

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```

*****
*
*   CASREACT now has more than 10 million reactions
*
*****

```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance

identification.

=> d que nos L32

```

L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL  L14
L23          STR
L25          16 SEA FILE=REGISTRY SUB=L18  SSS FUL  L23
L30          3 SEA FILE=CASREACT ABB=ON  PLU=ON  L25/PRO
L31          33 SEA FILE=CASREACT ABB=ON  PLU=ON  L18/RRT
L32          1 SEA FILE=CASREACT ABB=ON  PLU=ON  L31 (L) L30

```

=> file caplus

FILE 'CAPLUS' ENTERED AT 10:38:08 ON 22 MAR 2006  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Mar 2006 VOL 144 ISS 13  
 FILE LAST UPDATED: 21 Mar 2006 (20060321/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>  
 'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d que nos L26

```

L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL  L14
L23          STR
L25          16 SEA FILE=REGISTRY SUB=L18  SSS FUL  L23
L26          14 SEA FILE=CAPLUS ABB=ON  PLU=ON  L25

```

=> d que nos L27

```

L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL  L14
L23          STR
L25          16 SEA FILE=REGISTRY SUB=L18  SSS FUL  L23
L27          10 SEA FILE=CAPLUS ABB=ON  PLU=ON  L25 (L) PREP/RL

```

=> d que nos L29

```

L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS

```

L18 1954 SEA FILE=REGISTRY SUB=L16 SSS FUL L14  
L23 STR  
L25 16 SEA FILE=REGISTRY SUB=L18 SSS FUL L23  
L27 10 SEA FILE=CAPLUS ABB=ON PLU=ON L25 (L) PREP/RL  
L28 90 SEA FILE=CAPLUS ABB=ON PLU=ON L18 (L) (RCT OR RGT OR  
RACT)/RL  
L29 9 SEA FILE=CAPLUS ABB=ON PLU=ON L27 AND L28

=> s L26 or L27 or L29

L46 14 L26 OR L27 OR L29

=> d ibib abs hit L32 1; d ibib abs hitind hitstr L46 1-14

YOU HAVE REQUESTED DATA FROM FILE 'CASREACT' - CONTINUE? (Y)/N:y

L32 ANSWER 1 OF 1 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:36499 CASREACT

TITLE: Cyclopropyl building blocks in organic synthesis. 84.  
A new and productive route to 1-heteroarylcylopropanols

AUTHOR(S): Belov, Vladimir N.; Savchenko, Andrei I.; Sokolov, Viktor V.; Straub, Alexander; de Meijere, Armin

CORPORATE SOURCE: Institut fur Organische Chemie, Georg-August-Universitat Gottingen, Gottingen, 37077, Germany

SOURCE: European Journal of Organic Chemistry (2003), (3), 551-561

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

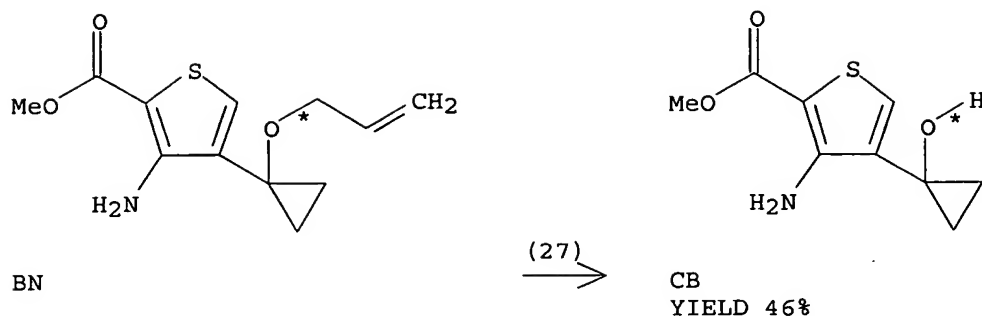
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Methoxy[(alkoxy)cyclopropyl]propenenitrile derivs. were designed and prepared from Et cyclopropylidenacetate as a valuable precursor to various 1-heteroarylcylopropanols. The key intermediates in this study included 3-methoxy-2-[1-[(4-methoxyphenyl)methoxy]cyclopropyl]-2-propenenitrile and 3-methoxy-2-[1-[(2-propenyl)oxy]cyclopropyl]-2-propenenitrile (I). Condensation of I with amidines, guanidine, hydrazine, and Me thioglycolate and subsequent removal of the allyl protecting group yields 1-heteroarylcylopropanols such as 1-[4-amino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]cyclopropanol (BAY 41-2272 metabolite II). II is a known very potent NO-independent stimulator of soluble guanylate cyclase. Direct cleavage of the allyl ether protecting group by palladium-catalyzed substitution with lithium p-toluenesulfinate in AcOH or treatment with cyclohexylmagnesium bromide/Ti(OiPr)<sub>4</sub> gives highly functionalized, sterically congested 1-heteroarylcylopropanols with intact amino and ester groups.

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(27) OF 128 ...BN ==> CB



RX(27) RCT BN 540134-38-1

STAGE(1)

RGT D 546-68-9 Ti(OPr-i)<sub>4</sub>, BI 931-50-0 Magnesium,  
bromocyclohexyl-  
SOL 60-29-7 Et<sub>2</sub>O, 109-99-9 THF  
CON SUBSTAGE(1) 4 hours, room temperature  
SUBSTAGE(2) overnight, room temperature

STAGE(2)

RGT CC 12125-02-9 NH<sub>4</sub>Cl  
SOL 7732-18-5 Water, 141-78-6 AcOEt  
CON room temperature

PRO CB 540134-72-3

NTE Grignard reaction

L46 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:20484 CAPLUS

TITLE: Synthesis of Thieno[2,3-b]Pyridinones Acting as  
Cytoprotectants and as Inhibitors of [3H]Glycine  
Binding to the N-Methyl-D-aspartate (NMDA) Receptor

AUTHOR(S): Buchstaller, Hans-Peter; Siebert, Carsten D.;  
Steinmetz, Ralf; Frank, Ina; Berger, Michael L.;  
Gottschlich, Rudolf; Leibrock, Joachim; Krug, Michael;  
Steinhilber, Dieter; Noe, Christian R.

CORPORATE SOURCE: Institute of Pharmaceutical Chemistry, Johann Wolfgang  
Goethe University, Frankfurt/Main, D-60439, Germany

SOURCE: Journal of Medicinal Chemistry (2006), 49(3), 864-871  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The standard glycine site antagonist of the N-methyl-D-aspartate (NMDA) receptor, 3-phenyl-4-hydroxyquinolin-2(1H)-one (I), was used as a template for bioisostere benzene/thiophene exchange. Phenylacetylation of aminothiophene carboxylic acid Me esters and subsequent cyclization delivered the three possible thienopyridinone isomers. 4-Hydroxy-5-phenylthieno[2,3-b]pyridin-6(7H)-one, with the shortest distance between the sulfur and the nitrogen atom, was the most potent isomer (K<sub>i</sub> against the binding of [3H]glycine to rat membranes 16 μM), comparable in potency to the model quinolinone (I, 12 μM). Replacement

of the Ph substituent of I by a 2-thienyl residue resulted in a 2-5-fold loss in potency and was abandoned. In the thieno part of the thienopyridinone nucleus, the most successful substituents were halogen (Cl or Br) close to the sulfur atom and short alkyl chains at the other position (K<sub>i</sub> values between 5.8 and 10.5 nM). Introduction of a 3'-phenoxy moiety yielded several compds. with still higher potencies. Quant. structure-activity relationship (QSAR) calcns. resulted in a consistent interpretation of the potencies of most compds. Several of these 3'-phenoxy derivs. protected mouse fibroblast cell lines with transfected NMDA receptors from glutamate-induced toxicity. In addition, the authors report in vivo results for four of these compds.

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

IT 103-80-0, Phenylacetyl chloride 103-82-2, Phenylacetic acid 4506-71-2  
4651-81-4 4651-93-8 4651-98-3 19156-63-9 19369-53-0 22288-78-4  
32852-81-6, 3-Phenoxyphenylacetic acid 39098-97-0, 2-Thienylacetyl  
chloride 69363-85-5 86750-63-2, 3-Phenoxyphenylacetyl chloride  
185215-32-1 349662-66-4 349662-82-4 **349662-85-7**  
349662-93-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of thieno[2,3-b]pyridinones acting as cytoprotectants and as inhibitors of [3H]glycine binding to the N-methyl-D-aspartate (NMDA) receptor)

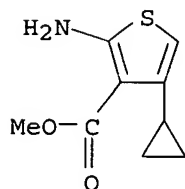
IT **349662-85-7**

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of thieno[2,3-b]pyridinones acting as cytoprotectants and as inhibitors of [3H]glycine binding to the N-methyl-D-aspartate (NMDA) receptor)

RN 349662-85-7 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-4-cyclopropyl-, methyl ester (9CI)  
(CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:423698 CAPLUS

DOCUMENT NUMBER: 142:458555

TITLE: Preparation of 2-aminothiophene derivatives as fungicides

INVENTOR(S): Selles, Patrice; Wailes, Jeffrey Steven; Whittingham, William Guy; Clarke, Eric Daniel

PATENT ASSIGNEE(S): Syngenta Participations A.-G., Switz.; Syngenta Limited

SOURCE: PCT Int. Appl., 155 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:



PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005044008	A2	20050519	WO 2004-GB4429	20041019
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:

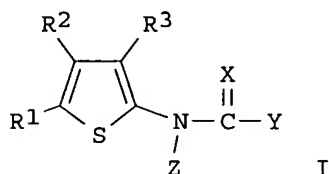
GB 2003-24653

A 20031022

OTHER SOURCE(S):

MARPAT 142:458555

GI



AB The 2-aminothiophene derivs. I [R1, R2 = H, halo, (cyclo)alkyl, hydroxyalkyl, etc.; R1R2= alkylene; R3 = H, halo, NO2, CN, (halo)alkyl, alkenyl, alkynyl, etc.; X = O, S, NH2, etc.; Y = H, (halo)alkyl, hydroxyalkyl, etc.; Z = H, (alkoxy)alkyl, alkylcarbonyl, etc.] are prepared as fungicides. The invention further relates to fungicidal compns. containing these compds., processes for preparing these compds. and to some of the compds. themselves.

ICM A01N043-10

ICS A01N043-12; C07D333-68

CC 5-2 (Agrochemical Bioregulators)

Section cross-reference(s): 27

IT 4506-71-2P 4651-91-6P 4651-94-9P 4815-28-5P 7311-95-7P  
 17402-78-7P 18774-47-5P, 2-Aminobenzo[b]thiophene-3-carbonitrile  
 18859-28-4P 23917-22-8P 36860-48-7P 36860-49-8P 39974-20-4P  
 63332-21-8P 66066-39-5P 88796-28-5P 92932-02-0P 107815-98-5P  
 117642-16-7P 150986-82-6P 150986-83-7P 193537-14-3P 265650-25-7P  
 330819-87-9P 344747-99-5P 612504-40-2P 712262-13-0P 851443-05-5P  
 851443-06-6P 851443-07-7P 851443-08-8P 851443-09-9P 851443-10-2P  
 851443-11-3P 851443-12-4P 851443-13-5P 851443-14-6P 851443-15-7P  
**851443-16-8P** 851443-17-9P 851443-18-0P 851443-19-1P  
 851443-20-4P 851443-21-5P 851443-22-6P 851443-23-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate in preparation of 2-aminothiophene derivative fungicides)

IT **851443-16-8P**

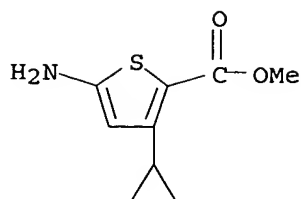
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate in preparation of 2-aminothiophene derivative fungicides)

RN 851443-16-8 CAPLUS

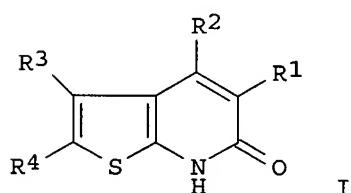
CN 2-Thiophenecarboxylic acid, 5-amino-3-cyclopropyl-, methyl ester (9CI)  
 (CA INDEX NAME)



L46 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:140804 CAPLUS  
 DOCUMENT NUMBER: 142:240419  
 TITLE: Preparation of substituted thieno[2,3-b]pyridones as activators for AMP-activated kinase for the treatment of diabetes and obesity  
 INVENTOR(S): Iyengar, Rajesh R.; Judd, Andrew S.; Zhao, Gang; Kym, Philip R.; Sham, Hing L.; Gu, Yugui; Liu, Gang; Liu, Mei; Zhao, Hongyu; Clark, Richard F.; Frevert, Ernst U.; Cool, Barbara L.; Zhang, Tianyuan; Keyes, Robert F.; Hansen, Todd M.; Xin, Zhili  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 86 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005038068	A1	20050217	US 2004-847144	20040517
PRIORITY APPLN. INFO.:			US 2003-471064P	P 20030516
OTHER SOURCE(S):	MARPAT	142:240419		

GI



AB Title compds. I [R1 = H, alkoxy, alkoxy carbonyl, etc.; R2 = alkoxy, OH, thioalkoxy, etc.; R3 = alkoxy carbonyl, aryl, etc.; R4 = H, alk(en/yn)yl, aryl, etc.] are prepared For instance, 3-(3,5-dimethylphenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile is prepared in several steps from 3,5-dimethylacetophenone, Et cyanoacetate and cyanoacetic acid. Representative compds. of the invention activate AMPK at a dose of 1-100  $\mu$ M. I are useful for the treatment of disorders such as diabetes, metabolic syndrome and obesity.

IC ICM C07D498-02  
 ICS A61K031-4743  
 INCL 514301000; 546114000

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 63

IT 844499-51-0P, 3-(4-Fluorophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-52-1P, 3-(4-Chlorophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-53-2P, 4-Hydroxy-6-oxo-3-[4-(trifluoromethyl)phenyl]-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-56-5P, 3-(4-Bromophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-58-7P, 3-(4'-Fluoro-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-65-6P, 2,5-Dichloro-3-(4-chlorophenyl)-4-hydroxythieno[2,3-b]pyridin-6(7H)-one 844499-66-7P, 4-Hydroxy-3-(4-nitrophenyl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-67-8P, 2-Bromo-4-hydroxy-3-(4-nitrophenyl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-68-9P, 3-(1,1'-Biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-69-0P, 4-Hydroxy-3-(2'-methyl-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-70-3P, 4-Hydroxy-3-(3'-methyl-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-71-4P, 4-Hydroxy-3-(2'-hydroxy-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-72-5P, 4-Hydroxy-3-(3'-hydroxy-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-73-6P, 4-Hydroxy-3-(2'-methoxy-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-74-7P, 4-Hydroxy-3-(3'-methoxy-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-75-8P, 4-Hydroxy-3-(4'-methoxy-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-76-9P, 3-(2'-Fluoro-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-77-0P, 3-(3'-Fluoro-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-78-1P, 3-(2'-Chloro-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-79-2P, 3-(3'-Chloro-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-80-5P, 3-(4'-Chloro-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-81-6P, 3-(4'-Cyano-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-82-7P, 3-(3'-Acetyl-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-83-8P, 3-[4'-(Dimethylamino)-1,1'-biphenyl-4-yl]-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-84-9P, 4-Hydroxy-6-oxo-3-(4'-phenoxy-1,1'-biphenyl-4-yl)-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-86-1P, 3-(4'-Acetyl-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844499-94-1P, 3-(4-Aminophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-02-3P, 2-Chloro-4-hydroxy-3-(4-bromophenyl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-03-4P, 2-Bromo-3-(5'-bromo-2'-hydroxy-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-05-6P, 3-(2'-Formyl-1,1'-biphenyl-4-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-06-7P, 4-Hydroxy-3-[4-(methoxymethoxy)phenyl]-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-11-4P, 4-Hydroxy-3-(4-hydroxyphenyl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-19-2P, 3-(3-Bromophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-29-4P, tert-Butyl [4-[5-(5-cyano-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridin-3-yl)thien-2-yl]phenyl]carbamate 844500-43-2P, 3-(5-Bromothien-2-yl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-46-5P, 3-[4-(Allyloxy)phenyl]-2-chloro-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-54-5P, 2-Chloro-4-hydroxy-3-[4-[(1-hydroxycyclopent-3-en-1-

yl)methoxy]phenyl]-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-72-7P, 4-Hydroxy-3-(5-iodo-4-methylthien-2-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-82-9P, Methyl 4-(2-chloro-5-cyano-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridin-3-yl)benzoate 844500-94-3P, 4-Hydroxy-3-[4-(4-hydroxybut-1-ynyl)phenyl]-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844501-05-9P, 7-[4-(5-Cyano-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridin-3-yl)phenyl]heptan-6-ynoic acid 844501-13-9P, 2-Chloro-4-hydroxy-6-oxo-3-(2-phenylcyclopropyl)-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844501-52-6P, 3-[4-(Allyloxy)phenyl]-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844501-62-8P, 3-[4-Bromo-5-(3-methoxyprop-1-ynyl)thiophen-2-yl]-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844501-74-2P, 4-Hydroxy-3-[4-(5-hydroxypent-1-ynyl)phenyl]-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844502-79-0P, Ethyl 4-hydroxy-3-(2'-hydroxy-1,1'-biphenyl-4-yl)-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carboxylate  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted thieno[2,3-b]pyridones as activators for AMP-activated kinase for treatment of diabetes and obesity)

IT 2079-53-0P, 1-(4-Allyloxyphenyl)ethanone 2089-23-8P, 1-(4-Allyloxyphenyl)propan-1-one 2887-72-1P 4815-32-1P, 2-Amino-5-methylthiophene-3-carboxylic acid ethyl ester 6739-22-6P, 1-(2-Phenylcyclopropyl)ethanone 7255-63-2P, 1-But-3-enylpyrrolidine 10537-63-0P, 1-(4-Vinylphenyl)ethanone 17044-70-1P, 3',5'-Dichloro-4'-hydroxyacetophenone 51828-69-4P, [4-(Acetyl)phenoxy]acetic acid ethyl ester 54696-05-8P, 4-Benzoyloxyacetophenone 58621-54-8P, 1-(3-Allyloxyphenyl)ethanone 70013-38-6P, 1-[5-(4-Hydroxyphenyl)thien-2-yl]ethanone 85699-00-9P, 1-(4-Methoxymethoxyphenyl)ethanone 120110-62-5P 147804-30-6P 160984-14-5P, (4-Acetylphenoxy)acetonitrile 306934-99-6P, 2-Amino-4-(4-bromophenyl)thiophene-3-carboxylic acid ethyl ester 590376-44-6P, 2-(2-Cyanoacetyl amino)-5-methylthiophene-3-carboxylic acid ethyl ester 837392-64-0P, 5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-dihydro-2H-indol-2-one 844499-49-6P, 2-Amino-4-(3,5-dimethylphenyl)thiophene-3-carboxylic acid ethyl ester 844499-50-9P, 2-(2-Cyanoacetyl amino)-4-(3,5-dimethylphenyl)thiophene-3-carboxylic acid ethyl ester 844499-62-3P, 4-(4-Chlorophenyl)-2-[[2-(ethoxycarbonyl)acetyl]amino]thiophene-3-carboxylic acid ethyl ester 844499-63-4P, 3-(4-Chlorophenyl)-4-hydroxy-7H-thieno[2,3-b]pyridin-6-one 844500-01-2P, 4-(4-Bromophenyl)-5-chloro-2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid ethyl ester 844500-24-9P, 2-Amino-4-(4-benzoyloxy-3,5-dichlorophenyl)thiophene-3-carboxylic acid ethyl ester 844500-25-0P, 4-(4-Benzoyloxy-3,5-dichlorophenyl)-2-[[2-(methoxycarbonyl)acetyl]amino]thiophene-3-carboxylic acid ethyl ester 844500-26-1P, 3-(3,5-Dichloro-4-benzoyloxyphenyl)-4-hydroxy-7H-thieno[2,3-b]pyridin-6-one 844500-32-9P, 3-[4-(2,3-Dimethoxyphenyl)phenyl]-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-35-2P, 2-Amino-4-(4-benzoyloxyphenyl)thiophene-3-carboxylic acid ethyl ester 844500-36-3P, 4-(4-Benzoyloxyphenyl)-2-[[2-(ethoxycarbonyl)acetyl]amino]thiophene-3-carboxylic acid ethyl ester 844500-37-4P, 3-(4-Benzoyloxyphenyl)-4-hydroxy-7H-thieno[2,3-b]pyridin-6-one 844500-38-5P, 3-(4-Hydroxyphenyl)-4-hydroxy-7H-thieno[2,3-b]pyridin-6-one 844500-41-0P, Ethyl 5'-amino-5-bromo-2,3'-bithiophene-4'-carboxylate 844500-42-1P, Ethyl 5-bromo-5'-[(cyanoacetyl)amino]-2,3'-bithiophene-4'-carboxylate 844500-51-1P, Ethyl 5'-amino-5-bromo-2'-chloro-2,3'-bithiophene-4'-carboxylate 844500-51-2P, Ethyl 5-bromo-2'-chloro-5'-[(cyanoacetyl)amino]-2,3'-bithiophene-4'-carboxylate 844500-52-3P, 3-(5-Bromothien-2-yl)-2-chloro-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-55-6P, 2-Cyano-3-[4-

[(ethoxycarbonyl)methoxy]phenyl]but-2-enoic acid ethyl ester  
 844500-56-7P, 2-Amino-4-[4-[(ethoxycarbonyl)methoxy]phenyl]thiophene-3-  
 carboxylic acid ethyl ester hydrochloride 844500-57-8P,  
 4-[4-[(2-Allyl-2-hydroxypent-4-enyl)oxy]phenyl]-2-aminothiophene-3-  
 carboxylic acid ethyl ester 844500-58-9P, 4-[4-[(2-Allyl-2-hydroxypent-4-  
 enyl)oxy]phenyl]-2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid ethyl  
 ester 844500-59-0P, 4-[4-[(2-Allyl-2-hydroxypent-4-enyl)oxy]phenyl]-5-  
 chloro-2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid ethyl ester  
 844500-60-3P, 5-Chloro-2-(2-cyanoacetyl amino)-4-[4-[(1-hydroxycyclopent-3-  
 enyl)methoxy]phenyl]thiophene-3-carboxylic acid ethyl ester  
 844500-77-2P, 2-Amino-4-[4-(2-hydroxy-2-methylpropoxy)phenyl]thiophene-3-  
 carboxylic acid ethyl ester 844500-78-3P, 4-[4-(2-Hydroxy-2-  
 methylpropoxy)phenyl]-2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid  
 ethyl ester 844500-79-4P, 4-[4-(2-Hydroxy-2-methylpropoxy)phenyl]-5-  
 chloro-2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid ethyl ester  
 844500-85-2P, 2-(2-Cyanoacetyl amino)-4-iodo-5-methylthiophene-3-carboxylic  
 acid ethyl ester 844500-86-3P, 4-Hydroxy-3-iodo-2-methyl-6-oxo-6,7-  
 dihydrothieno[2,3-b]pyridine-5-carbonitrile 844500-99-8P, tert-Butyl  
 4-[5-(5-cyano-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridin-3-yl)thien-2-  
 yl]-3,6-dihydropyridine-1(2H)-carboxylate 844501-01-5P,  
 2-Amino-4-(4-allyloxyphenyl)thiophene-3-carboxylic acid ethyl ester  
 844501-02-6P, 4-(4-Allyloxyphenyl)-2-(2-cyanoacetyl amino)thiophene-3-  
 carboxylic acid ethyl ester 844501-03-7P, 4-(4-Allyloxyphenyl)-5-chloro-  
 2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid ethyl ester  
 844501-14-0P, 2-Amino-4-(2-phenylcyclopropyl)thiophene-3-  
 carboxylic acid ethyl ester 844501-15-1P, 2-Cyano-3-(2-  
 phenylcyclopropyl)but-2-enoic acid ethyl ester 844501-16-2P,  
 2-(2-Cyanoacetyl amino)-4-(2-phenylcyclopropyl)thiophene-3-carboxylic acid  
 ethyl ester 844501-17-3P, 5-Chloro-2-(2-cyanoacetyl amino)-4-(2-  
 phenylcyclopropyl)thiophene-3-carboxylic acid ethyl ester 844501-21-9P,  
 4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)benzene-1,3-diol  
 844501-23-1P, 3-[3-(Allyloxy)phenyl]-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-  
 b]pyridine-5-carbonitrile 844501-27-5P, 5'-(Cyanoacetyl amino)-5-(pyridin-  
 2-yl)-[2,3']bithienyl-4'-carboxylic acid ethyl ester 844501-29-7P  
 844501-35-5P, N-[3-Fluoro-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-  
 yl)phenyl]acetamide 844501-37-7P, 4-Hydroxy-3-(4-hydroxymethylphenyl)-6-  
 oxo-3a,6,7,7a-tetrahydrothieno[2,3-b]pyridine-5-carbonitrile  
 844501-39-9P, 3-(4-Formylphenyl)-4-hydroxy-6-oxo-3a,6,7,7a-  
 tetrahydrothieno[2,3-b]pyridine-5-carbonitrile 844501-40-2P,  
 [[4-(5-Cyano-4-hydroxy-6-oxo-3a,6,7,7a-tetrahydrothieno[2,3-b]pyridin-3-  
 yl)benzylidene]amino]oxy]acetic acid 844501-57-1P, 1-[5-[4-  
 (Allyloxy)phenyl]thien-2-yl]ethanone 844501-58-2P, Ethyl  
 5-[4-(allyloxy)phenyl]-5'-amino-2,3'-bithiophene-4'-carboxylate  
 844501-59-3P, Ethyl 5-[4-(allyloxy)phenyl]-5'-[(cyanoacetyl amino)-2,3'-  
 bithiophene-4'-carboxylate 844501-63-9P, 3-(4-Bromo-5-iodothiophen-2-yl)-  
 4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile  
 844501-67-3P, 4-(4-Benzylloxy-3,5-dichlorophenyl)-2-(2-  
 cyanoacetyl amino)thiophene-3-carboxylic acid ethyl ester 844501-68-4P,  
 3-(4-Benzylloxy-3,5-dichlorophenyl)-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-  
 b]pyridine-5-carbonitrile 844501-78-6P, N-[3-Chloro-4-(4,4,5,5-  
 tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]acetamide 844501-80-0P,  
 2-[4-(2-Chloro-5-cyano-4-hydroxy-6-oxo-6,7-dihydrothieno[2,3-b]pyridin-3-  
 yl)phenoxy]acetic acid 844501-81-1P, 2-Amino-4-[4-  
 [(ethoxycarbonyl)methoxy]phenyl]-5-chlorothiophene-3-carboxylic acid ethyl  
 ester 844501-83-3P, 2-Cyano-3-(4-cyanomethoxyphenyl)-but-2-enoic acid  
 ethyl ester 844501-84-4P, 2-Amino-4-(4-cyanomethoxyphenyl)thiophene-3-  
 carboxylic acid ethyl ester 844501-85-5P, 2-(2-Cyanoacetyl amino)-4-(4-  
 cyanomethoxyphenyl)thiophene-3-carboxylic acid ethyl ester 844501-86-6P,  
 2-(2-Cyanoacetyl amino)-4-(4-cyanomethoxyphenyl)-5-chlorothiophene-3-  
 carboxylic acid ethyl ester 844501-92-4P, 2-(2-Cyanoacetyl amino)-4-(4-

nitrophenyl)thiophene-3-carboxylic acid ethyl ester 844501-93-5P,  
 2-(2-Cyanoacetyl amino)-4-(4-nitrophenyl)-5-chlorothiophene-3-carboxylic  
 acid ethyl ester 844501-94-6P, 2-(2-Cyanoacetyl amino)-4-(4-aminophenyl)-  
 5-chlorothiophene-3-carboxylic acid ethyl ester 844501-95-7P,  
 2-(2-Cyanoacetyl amino)-4-[4-(diallylamino)phenyl]-5-chlorothiophene-3-  
 carboxylic acid ethyl ester 844501-99-1P, 2-Amino-4-[4-  
 [(ethoxycarbonyl)methoxy]phenyl]thiophene-3-carboxylic acid ethyl ester  
 844502-01-8P, 4-(4-Acetylphenoxy)methyl)-4-hydroxypiperidine-1-carboxylic  
 acid tert-butyl ester 844502-02-9P, 4-[[[(4-(2-Cyano-2-(ethoxycarbonyl)-1-  
 methylethenyl)phenyl)oxy)methyl]-4-hydroxypiperidine-1-carboxylic acid  
 tert-butyl ester 844502-03-0P, 4-[[[4-[5-Amino-4-(ethoxycarbonyl)thiophen-  
 3-yl]phenoxy)methyl]-4-hydroxypiperidine-1-carboxylic acid tert-butyl  
 ester 844502-24-5P, 5'-(2-Cyanoacetyl amino)-5-iodo-4-  
 methyl[2,3']bithiophene-4'-carboxylic acid ethyl ester 844502-25-6P,  
 1-(5-Iodo-4-methylthiophene-2-yl)ethanone 844502-26-7P,  
 2-Cyano-3-(5-iodo-4-methylthiophene-2-yl)but-2-enoic acid ethyl ester  
 844502-27-8P, 5'-Amino-5-iodo-4-methyl-[2,3']bithiophene-4'-carboxylic  
 acid ethyl ester 844502-29-0P, tert-Butyl 5-acetylthiophene-2-  
 carboxylate 844502-30-3P 844502-31-4P, 5'-[(Cyanoacetyl)amino]-4'-  
 (ethoxycarbonyl)-2,2'-bithiophene-5-carboxylic acid 844502-32-5P, Ethyl  
 5-[(cyanoacetyl)amino]-5'-[[[2-(dimethylamino)ethyl]amino]carbonyl]-2,2'-  
 bithiophene-4-carboxylate 844502-42-7P, 4-(4-Allyloxyphenyl)-2-amino-5-  
 methylthiophene-3-carboxylic acid ethyl ester 844502-43-8P,  
 4-(4-Allyloxyphenyl)-2-(2-cyanoacetyl amino)-5-methylthiophene-3-carboxylic  
 acid ethyl ester 844502-47-2P, 1-(4-Benzyloxy-3,5-dibromophenyl)ethanone  
 844502-48-3P, 2-Amino-4-(4-benzyloxy-3,5-dibromophenyl)thiophene-3-  
 carboxylic acid ethyl ester 844502-49-4P, 4-(4-Benzyloxy-3,5-  
 dibromophenyl)-2-(2-cyanoacetyl amino)thiophene-3-carboxylic acid ethyl  
 ester 844502-50-7P, 3-(4-Benzyloxy-3,5-dibromophenyl)-4-hydroxy-6-oxo-  
 6,7-dihydrothieno[2,3-b]pyridine-5-carbonitrile 844502-57-4P,  
 5-Acetyl-N-methoxy-N-methylthiophene-2-carboxamide 844502-58-5P, Ethyl  
 5-amino-5'-[[methoxy(methyl)amino]carbonyl]-2,2'-bithiophene-4-carboxylate  
 844502-59-6P, Ethyl 5'-acetyl-5-amino-2,2'-bithiophene-4-carboxylate  
 844502-60-9P, Ethyl 5'-acetyl-5-[(cyanoacetyl)amino]-2,2'-bithiophene-4-  
 carboxylate 844502-61-0P, 2-(5-Acetylthien-2-yl)-4-hydroxy-6-oxo-6,7-  
 dihydrothieno[2,3-b]pyridine-5-carbonitrile 844502-63-2P 844502-64-3P  
 844502-65-4P, 2-[(tert-Butoxycarbonyl)amino]-4-(hydroxymethyl)thiophene-3-  
 carboxylic acid ethyl ester 844502-66-5P, 2-[(tert-Butoxycarbonyl)amino]-  
 4-formylthiophene-3-carboxylic acid ethyl ester 844502-67-6P,  
 2-[(tert-Butoxycarbonyl)amino]-4-(2-phenylvinyl)thiophene-3-carboxylic  
 acid ethyl ester 844502-68-7P, 2-Amino-4-styrylthiophene-3-carboxylic  
 acid ethyl ester 844502-69-8P, 2-(2-Cyanoacetyl amino)-4-(2-  
 phenylethenyl)thiophene-3-carboxylic acid ethyl ester 844502-71-2P,  
 2-[(tert-Butoxycarbonyl)amino]-4-ethynylthiophene-3-carboxylic acid ethyl  
 ester 844502-72-3P, 2-Amino-4-ethynylthiophene-3-carboxylic acid ethyl  
 ester 844502-73-4P, 2-Amino-4-(phenylethynyl)thiophene-3-carboxylic acid  
 ethyl ester 844502-74-5P, 2-(2-Cyanoacetyl amino)-4-  
 (phenylethynyl)thiophene-3-carboxylic acid ethyl ester 844502-80-3P,  
 4-(4-Bromophenyl)-2-[[2-(ethoxycarbonyl)acetyl]amino]thiophene-3-  
 carboxylic acid ethyl ester 844502-81-4P, 3-(4-Bromophenyl)-4-hydroxy-6-  
 oxo-6,7-dihydrothieno[2,3-b]pyridine-5-carboxylic acid ethyl ester  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of substituted thieno[2,3-b]pyridones as activators for  
 AMP-activated kinase for treatment of diabetes and obesity)

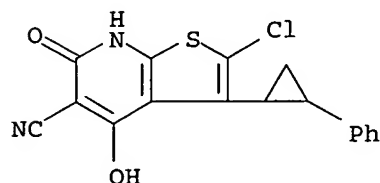
IT 844501-13-9P, 2-Chloro-4-hydroxy-6-oxo-3-(2-phenylcyclopropyl)-6,7-  
 dihydrothieno[2,3-b]pyridine-5-carbonitrile

RL: PAC (Pharmacological activity); RCT (Reactant); SPN  
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
 PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of substituted thieno[2,3-b]pyridones as activators for  
AMP-activated kinase for treatment of diabetes and obesity)

RN 844501-13-9 CAPLUS

CN Thieno[2,3-b]pyridine-5-carbonitrile, 2-chloro-6,7-dihydro-4-hydroxy-6-oxo-  
3-(2-phenylcyclopropyl)- (9CI) (CA INDEX NAME)



IT 844501-14-0P, 2-Amino-4-(2-phenylcyclopropyl)thiophene-3-  
carboxylic acid ethyl ester 844501-16-2P, 2-(2-Cyanoacetylamino)-  
4-(2-phenylcyclopropyl)thiophene-3-carboxylic acid ethyl ester

844501-17-3P, 5-Chloro-2-(2-cyanoacetylamino)-4-(2-  
phenylcyclopropyl)thiophene-3-carboxylic acid ethyl ester

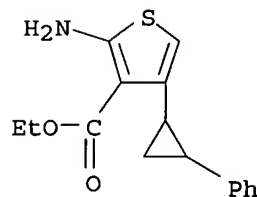
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of substituted thieno[2,3-b]pyridones as activators for  
AMP-activated kinase for treatment of diabetes and obesity)

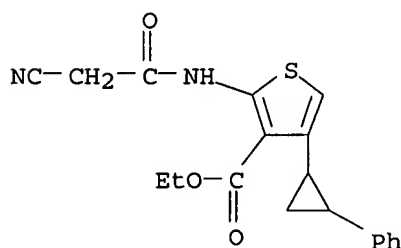
RN 844501-14-0 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-4-(2-phenylcyclopropyl)-, ethyl ester  
(9CI) (CA INDEX NAME)



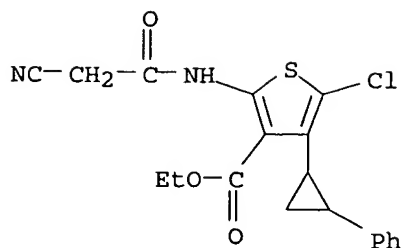
RN 844501-16-2 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-[(cyanoacetyl)amino]-4-(2-phenylcyclopropyl)-  
, ethyl ester (9CI) (CA INDEX NAME)

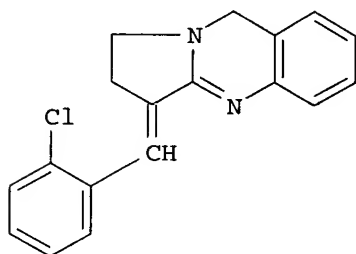


RN 844501-17-3 CAPLUS

CN 3-Thiophenecarboxylic acid, 5-chloro-2-[(cyanoacetyl)amino]-4-(2-  
phenylcyclopropyl)-, ethyl ester (9CI) (CA INDEX NAME)



L46 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:74680 CAPLUS  
 DOCUMENT NUMBER: 142:212050  
 TITLE: Pyrrolidinohydroquinazolines--a novel class of CCR3 modulators  
 AUTHOR(S): Anderskewitz, Ralf; Bauer, Rolf; Bodenbach, Gisela; Gester, Dirk; Gramlich, Bernd; Morschhaeuser, Gerd; Birke, Franz W.  
 CORPORATE SOURCE: Boehringer Ingelheim Pharma GmbH and Co. KG, Biberach an der Riss, D-88397, Germany  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(3), 669-673  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:212050  
 GI



I

AB A novel class of CCR3 modulators is described. Starting with lead compound I (Ki: 110 nM), which turned out to be an antagonist of eotaxin at the CCR3 receptor, further optimization led to compound 8b (Ki: 28 nM), which surprisingly proved to be an agonist.  
 CC 1-9 (Pharmacology)  
 Section cross-reference(s): 28  
 IT 83-38-5 89-98-5 96-48-0 104-50-7 123-11-5, reactions 446-52-6  
 447-61-0 613-69-4 695-06-7 874-42-0 1203-68-5,  
 [1,1'-Biphenyl]-2-carboxaldehyde 1424-66-4 1885-29-6 4403-69-4  
 4651-82-5 4651-91-6 4651-94-9 5098-11-3 5117-88-4 5264-35-7  
 6287-38-3 6630-33-7 10413-34-0 22927-13-5 24517-64-4 26260-02-6  
 51787-96-3 58124-28-0 84194-36-5 94651-33-9 841251-11-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)



(pyrrolidinohydroquinazolines: preparation and CCR3 receptor modulation)

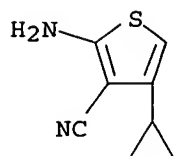
IT 58124-28-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(pyrrolidinohydroquinazolines: preparation and CCR3 receptor modulation)

RN 58124-28-0 CAPLUS

CN 3-Thiophenecarbonitrile, 2-amino-4-cyclopropyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:390242 CAPLUS

DOCUMENT NUMBER: 140:406731

TITLE: Preparation of N-(cyclopropylthienyl)carboxamides as fungicides

INVENTOR(S): Ehrenfreund, Josef; Tobler, Hans; Walter, Harald

PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

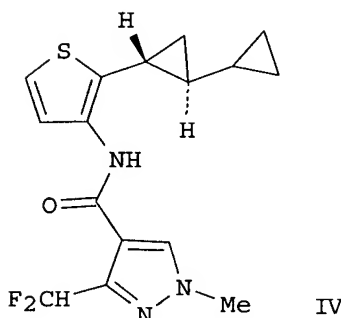
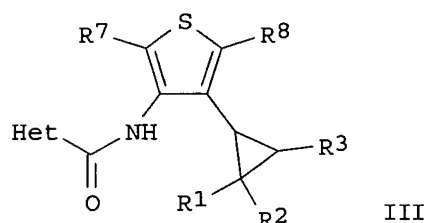
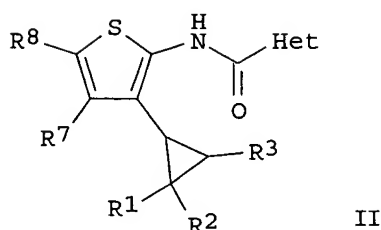
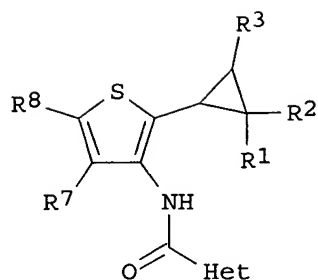
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039799	A1	20040513	WO 2003-EP11805	20031024
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2501739	AA	20040513	CA 2003-2501739	20031024
AU 2003286140	A1	20040525	AU 2003-286140	20031024
EP 1556377	A1	20050727	EP 2003-776869	20031024
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003015857	A	20050920	BR 2003-15857	20031024
JP 2006508089	T2	20060309	JP 2004-547558	20031024
US 2006030567	A1	20060209	US 2005-532847	20050427
PRIORITY APPLN. INFO.:			GB 2002-25554	A 20021101
			WO 2003-EP11805	W 20031024
OTHER SOURCE(S):			MARPAT 140:406731	
GI				



AB A fungicidally active compound I, II, or III [wherein Het = (un)substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole; R1 and R2 = independently H, halo, or Me; R3 = (un)substituted (cyclo)alkyl, alkenyl, alkynyl, Ph, heterocyclyl; R7 and R8 = independently H, halo, or (halo)alkyl] were prepared for use as active ingredients in agricultural or horticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl)thiophen-3-yl]amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH<sub>2</sub>Cl<sub>2</sub> to give trans-IV (97% purity). The latter showed excellent activity against *Puccinia recondita* on wheat (0-5% infestation) and showed good activity against *Podosphaera leucotricha* on apple, *Venturia inaequalis* on apple, *Erysiphe graminis* on barley, *Pyrenophora teres* on barley, *Alternaria solani* on tomato, and *Uncinula necator* on grape (<20% infestation for each).

IC ICM C07D409-12

ICS C07D411-12; C07D417-12; C07D333-36; A01N043-56; A01N043-36; A01N043-78; A01N043-40; A01N043-32

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 10

IT 688326-41-2P	688326-42-3P	688326-43-4P	688326-44-5P	688326-45-6P
688326-46-7P	688326-47-8P	688326-48-9P	688326-49-0P	688326-50-3P
688326-51-4P	688326-52-5P	688326-53-6P	688326-54-7P	688326-55-8P
688326-56-9P	688326-57-0P	688326-58-1P	688326-59-2P	688326-60-5P
688326-61-6P	688326-62-7P	688326-63-8P	688326-64-9P	688326-65-0P
688326-67-2P	688326-68-3P	688326-69-4P	688326-70-7P	688326-71-8P
688326-72-9P	688326-73-0P	688326-74-1P	688326-75-2P	688326-76-3P
688326-77-4P	688326-78-5P	688326-79-6P	688326-80-9P	688326-81-0P
688326-82-1P	688326-83-2P	688326-84-3P	688326-85-4P	688326-86-5P

688326-87-6P 688326-88-7P 688326-89-8P 688326-90-1P 688326-91-2P  
 688326-92-3P 688326-94-5P 688326-96-7P 688326-98-9P 688327-00-6P  
 688327-02-8P 688327-04-0P 688327-06-2P 688327-08-4P 688327-10-8P  
 688327-12-0P 688327-14-2P 688327-16-4P 688327-18-6P 688327-20-0P  
 688327-22-2P 688327-24-4P 688327-26-6P 688327-28-8P 688327-30-2P  
 688327-31-3P 688327-33-5P 688327-35-7P 688327-38-0P 688327-39-1P  
 688327-40-4P 688327-41-5P 688327-42-6P 688327-43-7P 688327-44-8P  
 688327-45-9P 688327-46-0P 688327-47-1P 688327-48-2P 688327-49-3P  
 688327-50-6P 688327-51-7P 688327-52-8P 688327-53-9P 688327-54-0P  
 688327-55-1P 688327-56-2P 688327-57-3P 688327-58-4P 688327-59-5P  
 688327-60-8P 688327-61-9P 688327-62-0P 688327-63-1P 688327-64-2P  
 688327-65-3P 688327-66-4P 688327-67-5P 688327-68-6P 688327-69-7P  
 688327-70-0P 688327-71-1P 688327-72-2P 688327-73-3P 688327-74-4P  
 688327-75-5P 688327-76-6P 688327-77-7P 688327-78-8P 688327-79-9P  
 688327-80-2P 688327-81-3P 688327-82-4P 688327-83-5P 688327-84-6P  
 688327-85-7P 688327-86-8P 688327-87-9P 688327-88-0P 688327-89-1P  
 688327-90-4P 688327-91-5P 688327-92-6P 688327-93-7P 688327-94-8P  
 688327-95-9P 688327-96-0P 688327-97-1P 688327-98-2P 688327-99-3P  
 688328-00-9P 688328-01-0P 688328-02-1P 688328-03-2P 688328-04-3P  
 688328-05-4P 688328-06-5P 688328-07-6P  
 688328-08-7P 688328-09-8P 688328-11-2P  
 688328-12-3P 688328-13-4P 688328-16-7P 688328-17-8P 688328-18-9P  
 688328-19-0P 688328-20-3P 688328-21-4P 688328-22-5P 688328-23-6P  
 688328-24-7P 688328-25-8P 688328-26-9P 688328-27-0P 688328-28-1P  
 688328-29-2P 688328-30-5P 688328-31-6P 688328-32-7P 688328-33-8P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP** (Preparation); USES (Uses)

(fungicide; preparation of N-(cyclopropylthienyl)carboxamides as fungicides)

IT 688328-34-9P, (2E)-3-(3-Bromothiophen-2-yl)-1-cyclopropylprop-2-en-1-one  
 688328-35-0P 688328-36-1P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (Preparation); **RACT** (Reactant or reagent)

(intermediate; preparation of N-(cyclopropylthienyl)carboxamides as fungicides)

IT 930-96-1, 3-Bromo-2-formylthiophene 1013-88-3, Benzophenonimine  
 112849-15-7, (Cyclopropylcarbonylmethyl)triphenylphosphonium bromide  
 176969-34-9, 3-Difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid  
 688328-37-2

RL: RCT (Reactant); **RACT** (Reactant or reagent)

(preparation of N-(cyclopropylthienyl)carboxamides as fungicides)

IT 688328-06-5P 688328-07-6P 688328-08-7P  
 688328-09-8P 688328-11-2P

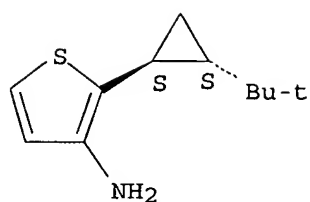
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP** (Preparation); USES (Uses)

(fungicide; preparation of N-(cyclopropylthienyl)carboxamides as fungicides)

RN 688328-06-5 CAPLUS

CN 3-Thiophenamine, 2-[(1R,2R)-2-(1,1-dimethylethyl)cyclopropyl]-, rel- (9CI)  
 (CA INDEX NAME)

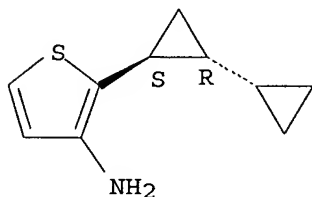
Relative stereochemistry.



RN 688328-07-6 CAPLUS

CN 3-Thiophenamine, 2-(1R,2S)-[1,1'-bicyclopropyl]-2-yl-, rel- (9CI) (CA INDEX NAME)

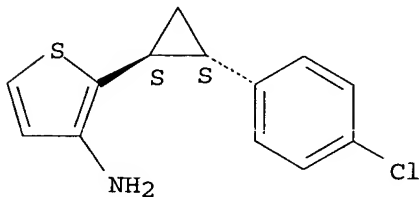
Relative stereochemistry.



RN 688328-08-7 CAPLUS

CN 3-Thiophenamine, 2-[(1R,2R)-2-(4-chlorophenyl)cyclopropyl]-, rel- (9CI) (CA INDEX NAME)

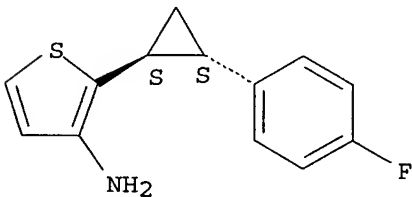
Relative stereochemistry.



RN 688328-09-8 CAPLUS

CN 3-Thiophenamine, 2-[(1R,2R)-2-(4-fluorophenyl)cyclopropyl]-, rel- (9CI) (CA INDEX NAME)

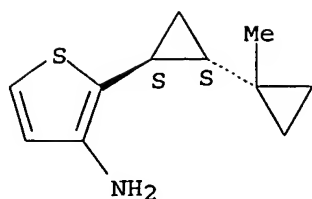
Relative stereochemistry.



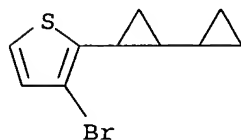
RN 688328-11-2 CAPLUS

CN 3-Thiophenamine, 2-[(1R,2R)-1'-methyl[1,1'-bicyclopropyl]-2-yl]-, rel- (9CI) (CA INDEX NAME)

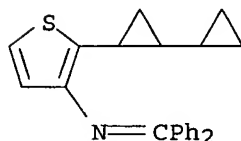
Relative stereochemistry.



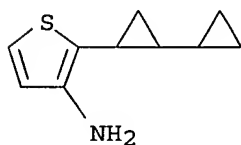
IT 688328-35-0P 688328-36-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of N-(cyclopropylthienyl)carboxamides as  
 fungicides)  
 RN 688328-35-0 CAPLUS  
 CN Thiophene, 2-[1,1'-bicyclopropyl]-2-yl-3-bromo- (9CI) (CA INDEX NAME)



RN 688328-36-1 CAPLUS  
 CN 3-Thiophenamine, 2-[1,1'-bicyclopropyl]-2-yl-N-(diphenylmethylene)- (9CI)  
 (CA INDEX NAME)



IT 688328-37-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of N-(cyclopropylthienyl)carboxamides as fungicides)  
 RN 688328-37-2 CAPLUS  
 CN 3-Thiophenamine, 2-[1,1'-bicyclopropyl]-2-yl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:109219 CAPLUS  
 DOCUMENT NUMBER: 139:36499  
 TITLE: Cyclopropyl building blocks in organic synthesis. 84.  
 A new and productive route to 1-

heteroaryl cyclopropanols

AUTHOR(S): Belov, Vladimir N.; Savchenko, Andrei I.; Sokolov, Viktor V.; Straub, Alexander; de Meijere, Armin

CORPORATE SOURCE: Institut für Organische Chemie, Georg-August-Universität Göttingen, Göttingen, 37077, Germany

SOURCE: European Journal of Organic Chemistry (2003), (3), 551-561

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:36499

AB Methoxy[(alkoxy)cyclopropyl]propenenitrile derivs. were designed and prepared from Et cyclopropylidenacetate as a valuable precursor to various 1-heteroaryl cyclopropanols. The key intermediates in this study included 3-methoxy-2-[1-[(4-methoxyphenyl)methoxy]cyclopropyl]-2-propenenitrile and 3-methoxy-2-[1-[(2-propenyl)oxy]cyclopropyl]-2-propenenitrile (I). Condensation of I with amidines, guanidine, hydrazine, and Me thioglycolate and subsequent removal of the allyl protecting group yields 1-heteroaryl cyclopropanols such as 1-[4-amino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]cyclopropanol (BAY 41-2272 metabolite II). II is a known very potent NO-independent stimulator of soluble guanylate cyclase. Direct cleavage of the allyl ether protecting group by palladium-catalyzed substitution with lithium p-toluenesulfinate in AcOH or treatment with cyclohexylmagnesium bromide/Ti(OiPr)<sub>4</sub> gives highly functionalized, sterically congested 1-heteroaryl cyclopropanols with intact amino and ester groups.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 128312-82-3P, 1-(2-Bromoethyl)cyclopropanol 540133-51-5P 540133-55-9P  
 540133-68-4P, 1-[(4-Methoxyphenyl)methoxy]cyclopropaneacetic acid  
 540133-73-1P, 1-(2-Propenyloxy)cyclopropaneacetic acid 540133-77-5P,  
 1-[(4-Methoxyphenyl)methoxy]cyclopropaneacetamide 540133-81-1P,  
 1-(2-Propenyloxy)cyclopropaneacetamide 540133-86-6P,  
 1-[(4-Methoxyphenyl)methoxy]cyclopropaneacetonitrile 540133-90-2P,  
 1-(2-Propenyloxy)cyclopropaneacetonitrile 540133-94-6P 540133-98-0P,  
 3-Methoxy-2-[1-[(4-methoxyphenyl)methoxy]cyclopropyl]-2-propenenitrile  
 540134-03-0P, 3-Methoxy-2-[1-[(2-propenyl)oxy]cyclopropyl]-2-  
 propenenitrile 540134-07-4P 540134-11-0P 540134-27-8P 540134-35-8P  
 540134-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [(amino)pyrimidinyl]cyclopropanol derivs. and analogs from methoxy[(alkoxy)cyclopropyl]propenenitrile derivs. as key intermediates)

IT 74592-36-2P, (Cyclopropylidene)acetic acid ethyl ester 256376-24-6DP,  
 BAY 41-2272, metabolite 540133-59-3P 540133-63-9P 540134-15-4P  
 540134-20-1P 540134-23-4P 540134-31-4P 540134-44-9P 540134-49-4P  
 540134-55-2P 540134-60-9P 540134-64-3P 540134-68-7P  
 540134-72-3P 540134-76-7P 540134-79-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

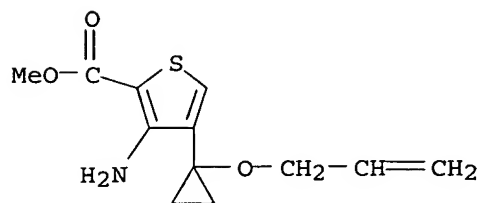
(preparation of [(amino)pyrimidinyl]cyclopropanol derivs. and analogs from methoxy[(alkoxy)cyclopropyl]propenenitrile derivs. as key intermediates)

IT 540134-38-1P

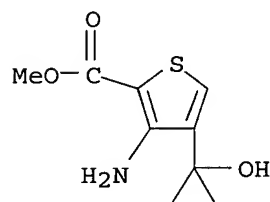
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [(amino)pyrimidinyl]cyclopropanol derivs. and analogs from methoxy[(alkoxy)cyclopropyl]propenenitrile derivs. as key intermediates)

RN 540134-38-1 CAPLUS  
 CN 2-Thiophenecarboxylic acid, 3-amino-4-[1-(2-propenyloxy)cyclopropyl]-, methyl ester (9CI) (CA INDEX NAME)



IT 540134-72-3P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (preparation of [(amino)pyrimidinyl]cyclopropanol derivs. and analogs from methoxy[(alkoxy)cyclopropyl]propenenitrile derivs. as key intermediates)  
 RN 540134-72-3 CAPLUS  
 CN 2-Thiophenecarboxylic acid, 3-amino-4-(1-hydroxycyclopropyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:504794 CAPLUS  
 DOCUMENT NUMBER: 137:63255  
 TITLE: Preparation of thieno[2,3-d]pyrimidine derivatives as cyclin-dependent kinase 4 (Cdk4) inhibitors having antitumor activity owing to cell cycle regulation  
 INVENTOR(S): Uoto, Kouichi; Horiuchi, Takao; Akabane, Kouichi; Takeda, Yasuyuki  
 PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 241 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002051849	A1	20020704	WO 2001-JP11354	20011225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,				

UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,  
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

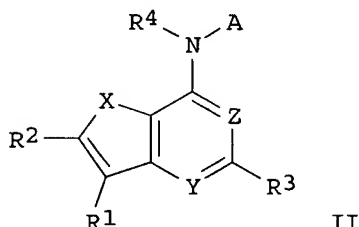
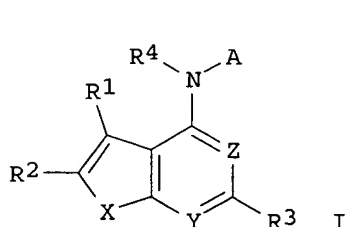
JP 2000-394169

A 20001226

OTHER SOURCE(S):

MARPAT 137:63255

GI



AB Compds. of the general formula (I) or (II) or salts thereof: [wherein X = S, O, NR5 (wherein R5 = H, alkyl); Y = N, CH; Z = N, CR6 (wherein R6 = H, halo, alkyl, etc.); R1, R2 = H, alkyl, alkoxy, alkenyl, alkynyl, aryl, aralkyl, acyl, mercapto, alkylthio, alkylsulfinyl, alkylsulfonyl, amino, mono- or dialkylamino, CONH2, mono- or dialkylcarbonyl, or R1 and R2 are linked to each other to form an (un)substituted 3- to 7-membered hydrocarbon or heterocyclic ring; R3 = H, (un)substituted alkyl or aryl; R4 = H, (un)substituted alkyl; and A is a group represented by the general formula -N:CR7R8, Q, Q1 [wherein R7 = H, (un)substituted alkyl; R8 = (un)substituted alkyl, aryl, or heterocyclyl; ring B = aryl or heteroaryl ring condensed to cyclohexane ring]] are prepared. Thus, to a solution of 6-tert-butyl-4-hydrazinothieno[2,3-d]pyrimidine ad in anhydrous benzene was added anhydrous Na2SO4 and heated at 100° with stirring for 2.5 h 1-(2-formylthiazol-4-ylmethyl)ethylcarbamic acid tert-Bu ester to give, after deprotection, 4-(1-aminoethyl)thiazole-2-carboxaldehyde N-[6-tert-butylthieno[2,3-d]pyrimidin-4-yl]hydrazone dihydrochloride (III). III showed IC50 of 0.019 and 0.83 µg/mL against Cdk4 and Cdk2, resp.

IC ICM C07D495-04

ICS C07D519-00; A61K031-519; A61K031-5377; A61P043-00; A61P035-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 7

IT 1119-16-0P, 4-Methylpentanal 1206-37-7P, 4-[(N,N-Dimethylamino)sulfonyl]benzoic acid 1823-90-1P, 3,3-Dimethyl-4-hydroxybutan-2-one 1849-53-2P, 3-Methoxy-2-pyridinecarboxaldehyde 1849-55-4P, 3-Hydroxy-2-pyridinecarboxaldehyde 2417-73-4P, 2-(Bromomethyl)benzoic acid methyl ester 3364-80-5P, Thiazole-4-carboxaldehyde 4670-56-8P, 2-Hydroxy-4-methylbenzoic acid methyl ester 6059-29-6P, 3-Benzoyloxy-2-hydroxymethylpyridine 6436-59-5P, 2-Methylthiazole-4-carboxylic acid ethyl ester 7210-73-3P, 4-Methylthiazole-2-carboxylic acid ethyl ester 7326-73-0P 13750-68-0P, 4-Methylthiazole-2-carboxaldehyde 14346-24-8P 14527-43-6P, Ethyl thiazole-4-carboxylate 16229-26-8P 16234-10-9P, Thieno[3,2-d]pyrimidin-4(3H)-one 16269-66-2P, 4-Chlorothieno[3,2-d]pyrimidine 18002-00-1P 18153-53-2P, 4-[(N,N-Dimethylamino)methyl]benzoic acid methyl ester 18593-51-6P, 6-Ethylthieno[2,3-d]pyrimidin-4(3H)-one 18593-52-7P 18595-18-1P, 3-Amino-4-methylbenzoic acid methyl ester 19156-63-9P, 2-Amino-5-ethyl-3-thiophenecarboxylic acid methyl ester 19580-36-0P, 4-[(4-Methylpiperazino)sulfonyl]benzoic acid 19886-78-3P, 2-[(N,N-Dimethylamino)methyl]benzaldehyde 20485-41-0P,



4-Methylthiazole-5-carboxylic acid 20582-55-2P, 4-Methylthiazole-5-carboxylic acid ethyl ester 27151-66-2P, 3,3-Dimethylglutaric acid monomethyl ester 27913-99-1P, 4-(4-Methylpiperazino)benzaldehyde 28094-70-4P, 2-(2-Diazoacetyl)pyrrolidine-1-carboxylic acid benzyl ester 32812-23-0P, 2,2-Dimethyl-1,4-butanediol 36874-95-0P, 4-[(N,N-Dimethylamino)methyl]benzaldehyde 40106-45-4P 40493-18-3P 51359-79-6P, 4-[(1,3-Dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]benzaldehyde 51984-46-4P, (3-Methoxy-2-pyridyl)methanol 53651-72-2P, 2-Allyl-2-methylmalonic acid diethyl ester 54049-92-2P, N,N-Dimethyl-4-formylbenzenesulfonamide 56525-63-4P, 3-Chloro-4-methylbenzoic acid methyl ester 59886-68-9P, 4-(4-Methyl-piperazin-1-yl)pyridine-2-carboxaldehyde 59906-29-5P 70386-38-8P 77202-58-5P 80708-77-6P, 3-[(N,N-Dimethylamino)methyl]benzaldehyde 80783-13-7P, 3,3-Dimethyl-4-methoxybutan-2-one 81136-42-7P, 4-Chloro-6-ethylthieno[2,3-d]pyrimidine 82413-62-5P 82586-66-1P, 2-[(N,N-Dimethylamino)methyl]thiazole-4-carboxylic acid ethyl ester 86762-06-3P, 4-Chlorothieno[2,3-d]pyrimidine-6-carbonyl chloride 89999-70-2P, 3-[(N,N-Dimethylamino)methyl]benzoic acid methyl ester 94454-57-6P, 3-Benzoyloxy-2-formylpyridine 97547-16-5P, [2-(4-Methylthiazol-5-yl)ethyl]carbamic acid tert-butyl ester 106203-24-1P 106691-21-8P, 4-Chloro-6-methylthieno[2,3-d]pyrimidine 107834-36-6P, 2-Methyl-5-isoindolinecarboxaldehyde 108354-78-5P, 2-Amino-4,5,6,7-tetrahydro-1-benzothiophene-3-carboxylic acid methyl ester 108831-66-9P, 6-Methylthieno[2,3-d]pyrimidin-4(3H)-one 115954-27-3P, Dimethyl-[2-(4-methylthiazol-5-yl)ethyl]amine 123444-68-8P 123986-64-1P, N-(4-(Hydroxymethyl)benzyl)carbamic acid tert-butyl ester 127785-49-3P 132390-68-2P, N,N-Dimethyl-3-formylbenzenesulfonamide 144033-44-3P, 2-(t-Butyldimethylsilyloxy)-4-methylbenzoic acid methyl ester 149587-85-9P, 2-Amino-5-isopropyl-3-thiophenecarboxylic acid methyl ester 150058-64-3P, 2-(t-Butyldimethylsilyloxy)methyl-6-hydroxymethylpyridine 152998-85-1P, 4-Chloro-6-ethyl-2-methylthieno[2,3-d]pyrimidine 155087-22-2P, 4-[(2-Methoxy-2-oxoethyl)sulfanyl]thieno[2,3-d]pyrimidine-6-carboxylic acid methyl ester 156866-52-3P, (4-Formylbenzyl)carbamic acid tert-butyl ester 162084-83-5P, 2-(t-Butyldimethylsilyloxy)methyl-6-formylpyridine 164294-15-9P 174525-96-3P 186641-76-9P 186641-79-2P 195155-27-2P, 4-[(4-Methylpiperazino)sulfonyl]benzaldehyde 196880-47-4P, 4-[(t-Butyldiphenylsilyloxy)methyl]benzaldehyde 198995-11-8P, 4-Methyl-5-methoxy-4-methoxymethyl-pent-1-ene 199599-68-3P, 2-[(N,N-Dimethylamino)methyl]thiazole-4-carboxaldehyde 202594-99-8P 210410-11-0P 211942-97-1P, 4-Cyclopropylthiazole-2-carboxaldehyde 215928-65-7P, 6-(tert-Butyl)thieno[3,2-d]pyrimidin-4(3H)-one 216574-71-9P, 2-Amino-5-(tert-butyl)-3-thiophenecarboxylic acid methyl ester 222409-98-5P, 3-[(t-Butylamino)sulfonyl]benzoic acid 222410-08-4P, N-(tert-Butyl)-3-formylbenzenesulfonamide 243968-07-2P 243968-08-3P 243968-09-4P 253801-15-9P, 5-Formyl-1,3-dihydro-2H-isoindole-2-carboxylic acid tert-butyl ester 253801-18-2P 258353-46-7P, 2-Amino-4,7-dihydro-5H-thieno[2,3-c]pyran-3-carboxylic acid methyl ester 314268-40-1P, 4-[(4-Methylpiperazino)methyl]benzoic acid methyl ester 317358-83-1P 318471-43-1P 343855-83-4P, 2-Amino-5-(n-propyl)-3-thiophenecarboxylic acid methyl ester 350988-48-6P, 2-Amino-5-benzyl-3-thiophenecarboxylic acid methyl ester 365996-10-7P, 2-Formyl-6,7-dihydro[1,3]thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid tert-butyl ester 365996-59-4P, N,N-Dimethyl-N-(thiazol-5-yl)methylamine 371222-37-6P, 6-Formyl-3,4-dihydro-2(1H)-isoquinolinecarboxylic acid tert-butyl ester 415952-34-0P 439691-78-8P 439691-79-9P 439691-80-2P, 4-[(4-Methylpiperazino)methyl]benzaldehyde 439691-81-3P 439691-82-4P 439691-83-5P 439691-84-6P 439691-85-7P, 2-(5-(Hydroxymethyl)-1,3-dihydro-2H-isoindol-2-yl)acetic acid tert-butyl ester 439691-86-8P, 2-(5-Formyl-1,3-dihydro-2H-isoindol-2-yl)acetic acid

tert-butyl ester 439691-87-9P, 5-(Hydroxymethyl)-2-methylisoindoline  
 439691-88-0P, 2-Isopropyl-5-isoindolinecarboxaldehyde 439691-89-1P,  
 4-[(N,N-Dimethylamino)methyl]-3-fluorobenzoic acid methyl ester  
 439691-90-4P, 4-[(N,N-Dimethylamino)methyl]-3-fluorobenzaldehyde  
 439691-91-5P, 3-Chloro-4-[(N,N-dimethylamino)methyl]benzaldehyde  
 439691-92-6P, 2-(t-Butyldimethylsilyloxy)-4-[(N,N-  
 dimethylamino)methyl]benzoic acid methyl ester 439691-93-7P,  
 4-[(N,N-Dimethylamino)methyl]-2-hydroxybenzaldehyde 439691-94-8P,  
 N-(4-Formylbenzyl)-N-methylcarbamic acid tert-butyl ester 439691-95-9P  
 439691-96-0P, [4-(Azidomethyl)phenyl]methanol 439691-97-1P  
 439691-98-2P, 4-(1-Methyl-3-azetidiny)benzaldehyde 439691-99-3P,  
 6-[(E)-3-Ethoxy-3-oxo-1-propenyl]-3,4-dihydroisoquinoline-2(1H)-carboxylic  
 acid tert-butyl ester 439692-00-9P 439692-01-0P 439692-02-1P,  
 4-[(N,N-Dimethylamino)methyl]thiazole-2-carboxaldehyde 439692-03-2P,  
 5-[(N,N-Dimethylamino)methyl]thiazole-2-carboxaldehyde 439692-04-3P,  
 2-Formyl-5-methyl-4,5,6,7-tetrahydro[1,3]thiazolo[5,4-c]pyridine  
 439692-05-4P, 4-Cyclopropylthiazole-2-carboxylic acid ethyl ester  
 439692-06-5P 439692-07-6P, Methyl(4-methylthiazol-5-ylmethyl)carbamic  
 acid tert-butyl ester 439692-08-7P, Methyl(2-formyl-4-methylthiazol-5-  
 ylmethyl)carbamic acid tert-butyl ester 439692-09-8P,  
 Methyl(thiazol-4-ylmethyl)carbamic acid tert-butyl ester 439692-10-1P  
 439692-11-2P, Methyl(thiazol-5-ylmethyl)carbamic acid tert-butyl ester  
 439692-12-3P 439692-13-4P 439692-14-5P 439692-15-6P 439692-16-7P  
 439692-17-8P, [2-(2-Formyl-4-methylthiazol-5-yl)ethyl]carbamic acid  
 tert-butyl ester 439692-18-9P, Dimethyl-[2-(2-formyl-4-methylthiazol-5-  
 yl)ethyl]amine 439692-19-0P, Methyl(4-trifluoromethylthiazol-5-  
 ylmethyl)carbamic acid tert-butyl ester 439692-20-3P 439692-21-4P  
 439692-22-5P 439692-23-6P 439692-24-7P 439692-25-8P 439692-27-0P  
 439692-28-1P 439692-29-2P 439692-30-5P 439692-31-6P,  
 3-[2-(N-t-Butoxycarbonyl-N-methylamino)ethoxy]isoxazole-5-carboxaldehyde  
 439692-32-7P, 4-(5-Methoxycarbonylisoxazol-3-yloxy)piperidine-1-carboxylic  
 acid tert-butyl ester 439692-33-8P, 4-(5-Formylisoxazol-3-  
 yloxy)piperidine-1-carboxylic acid tert-butyl ester 439692-34-9P,  
 2-(Hydroxymethyl)-N-methylthiazole-4-carboxamide 439692-35-0P,  
 5-(4-Methylpiperazin-1-yl)thiophene-2-carboxaldehyde 439692-36-1P  
 439692-37-2P 439692-38-3P 439692-39-4P 439692-40-7P 439692-41-8P,  
 4-[[2-(N,N-Dimethylamino)ethyl]methylamino]-pyridine-2-carboxaldehyde  
 439692-42-9P 439692-43-0P 439692-44-1P 439692-45-2P 439692-46-3P  
 439692-47-4P, 2-(2-Bromoacetyl)pyrrolidine-1-carboxylic acid benzyl ester  
 439692-48-5P, 2-(2-Hydroxymethyl-4-thiazolyl)pyrrolidine-1-carboxylic acid  
 benzyl ester 439692-49-6P, 2-(2-Hydroxymethyl-4-thiazolyl)pyrrolidine-1-  
 carboxylic acid tert-butyl ester 439692-50-9P, 2-(2-Formyl-4-  
 thiazolyl)pyrrolidine-1-carboxylic acid tert-butyl ester 439692-51-0P  
 439692-52-1P, 4-Chloro-6-isopropylthieno[2,3-d]pyrimidine 439692-53-2P  
 439692-54-3P, 6-(tert-Butyl)thieno[2,3-d]pyrimidin-4(3H)-one 439692-55-4  
 P, 6-(tert-Butyl)-4-chlorothieno[2,3-d]pyrimidine 439692-56-5P  
 439692-57-6P, 2,2-Dimethyl-1-(t-butyldiphenylsilyloxy)-4-pentene  
 439692-58-7P, 3,3-Dimethyl-4-(t-butyldiphenylsilyloxy)butanal  
 439692-59-8P, 2-Amino-5-[2-(t-butyldiphenylsilyloxy)-1,1-dimethylethyl]-3-  
 thiophenecarboxylic acid methyl ester 439692-60-1P, 6-[2-(t-  
 Butyldiphenylsilyloxy)-1,1-dimethylethyl]thieno[2,3-d]pyrimidin-4(3H)-one  
 439692-61-2P 439692-62-3P, 6-Benzylthieno[2,3-d]pyrimidin-4(3H)-one  
 439692-63-4P, 6-Benzyl-4-chlorothieno[2,3-d]pyrimidine 439692-64-5P  
 439692-65-6P, 2-Amino-5-(1,3,3-trimethylbutyl)-3-thiophenecarboxylic acid  
 methyl ester 439692-66-7P, 6-(1,3,3-Trimethylbutyl)thieno[2,3-  
 d]pyrimidin-4(3H)-one 439692-67-8P, 4-Chloro-6-(1,3,3-  
 trimethylbutyl)thieno[2,3-d]pyrimidine 439692-68-9P 439692-69-0P  
 439692-70-3P, 6-Pentylthieno[2,3-d]pyrimidin-4(3H)-one 439692-71-4P,  
 4-Chloro-6-pentylthieno[2,3-d]pyrimidine 439692-72-5P 439692-73-6P,  
 2-Amino-5-isobutyl-3-thiophenecarboxylic acid methyl ester 439692-74-7P,

6-Isobutylthieno-[2,3-d]pyrimidin-4(3H)-one 439692-75-8P,  
 4-Chloro-6-isobutylthieno-[2,3-d]pyrimidine 439692-76-9P 439692-77-0P,  
 2-Amino-5-sec-butyl-3-thiophenecarboxylic acid methyl ester  
 439692-78-1P, 6-(sec-Butyl)thieno-[2,3-d]pyrimidin-4(3H)-one  
 439692-79-2P, 4-Chloro-6-(sec-butyl)thieno-[2,3-d]pyrimidine  
 439692-80-5P 439692-81-6P, 6-(n-Propyl)thieno-[2,3-d]pyrimidin-4(3H)-one  
 439692-82-7P, 4-Chloro-6-(n-propyl)thieno-[2,3-d]pyrimidine 439692-83-8P  
 439692-85-0P, 2-Amino-5-(1,5-dimethyl-4-hexenyl)-3-thiophenecarboxylic  
 acid methyl ester 439692-87-2P, 4-Chloro-6-(1,5-dimethyl-4-  
 hexenyl)thieno-[2,3-d]pyrimidine 439692-88-3P 439692-89-4P,  
 5-Ethyl-6-methylthieno[2,3-d]pyrimidin-4(3H)-one 439692-90-7P,  
 4-Chloro-5-ethyl-6-methylthieno[2,3-d]pyrimidine 439692-91-8P  
 439692-92-9P, 2-(Benzoylamino)-5-ethyl-3-thiophenecarboxamide  
 439692-93-0P, 6-Ethyl-4-hydrazino-2-phenylthieno[2,3-d]pyrimidine  
 439692-94-1P, N-Acetyl-2-(acetylamino)-5-ethyl-3-thiophenecarboxamide  
 439692-95-2P, 6-Ethyl-4-hydrazino-2-methylthieno[2,3-d]pyrimidine  
 439692-96-3P **439692-97-4P**, 2-Amino-5-cyclopropyl-3-  
 thiophenecarboxylic acid methyl ester **439692-98-5P**,  
 6-Cyclopropylthieno[2,3-d]pyrimidin-4(3H)-one **439692-99-6P**,  
 4-Chloro-6-cyclopropylthieno[2,3-d]pyrimidine **439693-00-2P**  
 439693-01-3P, 2-Amino-5-cyclobutyl-3-thiophenecarboxylic acid methyl ester  
 439693-02-4P, 6-Cyclobutylthieno[2,3-d]pyrimidin-4(3H)-one 439693-03-5P,  
 4-Chloro-6-cyclobutylthieno[2,3-d]pyrimidine 439693-04-6P  
 439693-05-7P, 4-Hydrazino-2-methylfuro[2,3-b]pyridine 439693-06-8P,  
 4-Hydrazino-2-methylfuro[3,2-c]pyridine 439693-07-9P,  
 4-Hydrazino-2-methylthieno[3,2-c]pyridine 439693-08-0P 439693-09-1P  
 439693-10-4P 439693-11-5P 439693-12-6P, 3,3-Dimethyl-5-morpholino-5-  
 oxopentanoic acid methyl ester 439693-13-7P, 3,3-Dimethyl-5-morpholino-1-  
 pentanol 439693-14-8P, 2-Amino-5-(1,1-dimethyl-3-  
 morpholinopropyl)thiophene-3-carboxylic acid methyl ester 439693-15-9P,  
 6-(1,1-Dimethyl-3-morpholinopropyl)thieno[2,3-d]pyrimidin-4-(3H)-one  
 439693-16-0P, 4-Chloro-6-(1,1-dimethyl-3-morpholinopropyl)thieno[2,3-  
 d]pyrimidine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)

(preparation of thieno[2,3-d]pyrimidine derivs. as cyclin-dependent kinase 4  
 (Cdk4) inhibitors having antitumor activity owing to cell cycle  
 regulation)

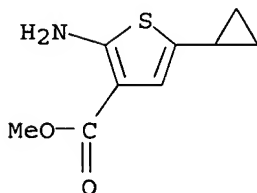
IT **439692-97-4P**, 2-Amino-5-cyclopropyl-3-thiophenecarboxylic acid  
 methyl ester **439692-98-5P**, 6-Cyclopropylthieno[2,3-d]pyrimidin-  
 4(3H)-one **439692-99-6P**, 4-Chloro-6-cyclopropylthieno[2,3-  
 d]pyrimidine **439693-00-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)

(preparation of thieno[2,3-d]pyrimidine derivs. as cyclin-dependent kinase 4  
 (Cdk4) inhibitors having antitumor activity owing to cell cycle  
 regulation)

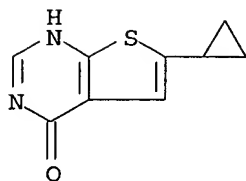
RN 439692-97-4 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-5-cyclopropyl-, methyl ester (9CI)  
 (CA INDEX NAME)



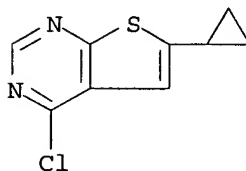
RN 439692-98-5 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(1H)-one, 6-cyclopropyl- (9CI) (CA INDEX NAME)



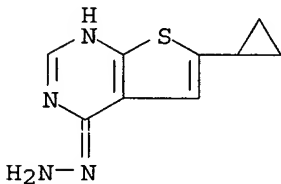
RN 439692-99-6 CAPLUS

CN Thieno[2,3-d]pyrimidine, 4-chloro-6-cyclopropyl- (9CI) (CA INDEX NAME)



RN 439693-00-2 CAPLUS

CN Thieno[2,3-d]pyrimidin-4(1H)-one, 6-cyclopropyl-, hydrazone (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:317056 CAPLUS

DOCUMENT NUMBER: 135:107200

TITLE: Synthesis of novel 2-aminothiophene-3-carboxylates by variations of the Gewald reaction

AUTHOR(S): Buchstaller, Hans-Peter; Siebert, Carsten D.; Lyssy, Ralf H.; Frank, Ina; Duran, Adil; Gottschlich, Rudolf; Noe, Christian R.

CORPORATE SOURCE: Merck KGaA, Darmstadt, D-64271, Germany

SOURCE: Monatshefte fuer Chemie (2001), 132(2), 279-293

CODEN: MOCMB7; ISSN: 0026-9247

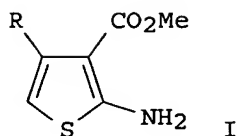
PUBLISHER: Springer-Verlag Wien

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:107200

GI



AB The synthesis of the title compds. through variations of the Gewald reaction is presented. Knoevenagel condensation of methylketone derivs. with Me cyanoacetate and subsequent treatment of the  $\alpha,\beta$ -unsatd. nitriles with sulfur and amine resulted in the corresponding 2-aminothiophenes I. Reaction of methylketone derivs. bearing a leaving group at the Me group under modified Gewald conditions selectively led to the formation of 4-substituted 2-aminothiophenes. The introduction of the sulfur atom occurs through nucleophilic displacement with sodium sulfide.

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

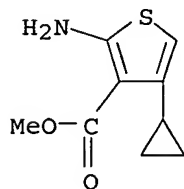
IT 10413-33-9P 349662-33-5P 349662-36-8P 349662-41-5P 349662-44-8P  
 349662-51-7P 349662-57-3P 349662-62-0P 349662-66-4P 349662-74-4P  
 349662-82-4P **349662-85-7P** 349662-93-7P 349662-96-0P  
 349663-00-9P 349663-04-3P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (synthesis of 2-aminothiophene-3-carboxylates by variations of the Gewald reaction)

IT **349662-85-7P**  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (synthesis of 2-aminothiophene-3-carboxylates by variations of the Gewald reaction)

RN 349662-85-7 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-4-cyclopropyl-, methyl ester (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L46 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:539272 CAPLUS

DOCUMENT NUMBER: 119:139272

TITLE: Thieno[2,3-b]pyrazine-2,3(1H,4H)-diones for treating psychiatric and neurological disorders

INVENTOR(S): Joergensen, Anker Steen; Faarup, Peter; Guddal, Erling; Jeppesen, Lone

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.

SOURCE: PCT Int. Appl., 80 pp.  
 CODEN: PIXXD2

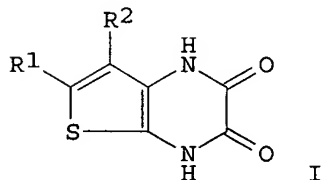
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9308197	A1	19930429	WO 1992-DK308	19921021
W: AU, BG, CA, CS, FI, HU, JP, KR, NO, PL, RO, RU				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
IL 103440	A1	19960331	IL 1992-103440	19921015
US 5284847	A	19940208	US 1992-962958	19921016
ZA 9208096	A	19940420	ZA 1992-8096	19921020
AU 9229025	A1	19930521	AU 1992-29025	19921021
AU 659243	B2	19950511		
EP 609371	A1	19940810	EP 1992-922930	19921021
EP 609371	B1	19960424		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
JP 06510789	T2	19941201	JP 1992-507363	19921021
JP 2519020	B2	19960731		
AT 137239	E	19960515	AT 1992-922930	19921021
ES 2088162	T3	19960801	ES 1992-922930	19921021
FI 9401877	A	19940422	FI 1994-1877	19940422
NO 9401476	A	19940622	NO 1994-1476	19940422
PRIORITY APPLN. INFO.:			DK 1991-1771	A 19911023
			WO 1992-DK308	A 19921021
OTHER SOURCE(S):		MARPAT 119:139272		
GI				



AB The title compds. I [R1 = H, (un)branched (un)substituted C1-6 alkyl, C2-6 alkenyl, C3-8 cycloalkyl, halogen, etc; R2 = H, (un)branched C1-6 alkyl, C2-6 alkenyl, C3-8 cycloalkyl, etc.], useful in treating central nervous system ailments, and which are potent and selective antagonists at the glycine-binding site on the NMDA receptor complex, are prepared, and pharmaceutical formulations containing them presented. Thus, Me 3-amino-4-methylthiophene-2-carboxylate was converted into I (R1 = H, R2 = Me) (II) in 4 steps. II demonstrated 50% increase in time to onset of NMDA-induced clonic seizures in mice of 7.0 µg/kg per min.

IC ICM C07D513-04

ICS A61K031-495

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

IT 17407-28-2P 53246-74-5P 53276-28-1P 68746-61-2P 72965-15-2P  
 72965-16-3P 93222-76-5P 101537-64-8P 120109-75-3P  
 125027-35-2P 149569-41-5P 149569-42-6P 149569-43-7P 149587-72-4P  
 149587-73-5P 149587-74-6P 149587-75-7P 149587-76-8P 149587-77-9P  
 149587-78-0P 149587-79-1P 149587-80-4P 149587-81-5P 149587-83-7P  
 149587-84-8P 149587-85-9P 149587-86-0P 149587-87-1P 149587-88-2P  
 149587-89-3P 149587-90-6P 149587-91-7P 149587-92-8P 149587-93-9P  
 149587-94-0P 149587-95-1P 149587-96-2P 149587-97-3P 149587-98-4P  
 149587-99-5P 149588-00-1P 149588-01-2P

149588-02-3P 149588-04-5P 149588-05-6P 149588-06-7P  
 149588-07-8P 149588-08-9P 149588-09-0P 149588-10-3P 149588-11-4P  
 149588-12-5P 149588-13-6P 149588-14-7P 149588-15-8P 149588-16-9P  
 149588-17-0P 149588-18-1P 149588-19-2P 149588-20-5P 149588-21-6P  
 149588-22-7P 149588-23-8P 149588-24-9P 149588-25-0P 149588-26-1P  
 149588-27-2P 149588-28-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of NMDA receptor antagonists)

IT 120109-75-3P 149588-00-1P 149588-01-2P

149588-02-3P

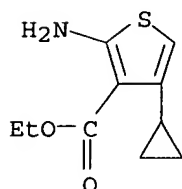
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of NMDA receptor antagonists)

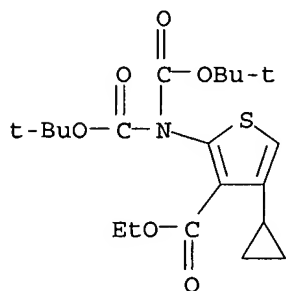
RN 120109-75-3 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-4-cyclopropyl-, ethyl ester (9CI) (CA INDEX NAME)



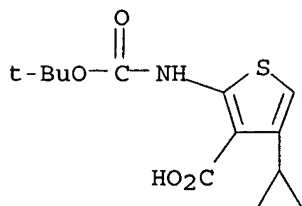
RN 149588-00-1 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-[bis[(1,1-dimethylethoxy)carbonyl]amino]-4-cyclopropyl-, ethyl ester (9CI) (CA INDEX NAME)

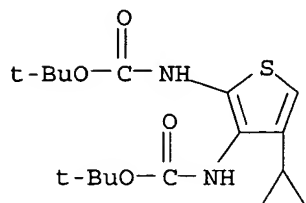


RN 149588-01-2 CAPLUS

CN 3-Thiophenecarboxylic acid, 4-cyclopropyl-2-[[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 149588-02-3 CAPLUS  
 CN Carbamic acid, (4-cyclopropyl-2,3-thiophenediyl)bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



L46 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:220744 CAPLUS

DOCUMENT NUMBER: 114:220744

TITLE: Structure-activity relationships for enhancement of adenosine A1 receptor binding by 2-amino-3-benzoylthiophenes

AUTHOR(S): Bruns, Robert F.; Fergus, James H.; Coughenour, Linda L.; Courtland, Geneva G.; Pugsley, Thomas A.; Dodd, John H.; Tinney, Francis J.

CORPORATE SOURCE: Dep. Pharmacol., Warner-Lambert Co., Ann Arbor, MI, 48105, USA

SOURCE: Molecular Pharmacology (1990), 38(6), 950-8

CODEN: MOPMA3; ISSN: 0026-895X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The structural requirements for stimulation of adenosine A1 agonist binding by 2-amino-3-benzoylthiophenes and related compds. were investigated. Slowing of the dissociation of N6-[3H]cyclohexyladenosine binding was used as a specific measure of the allosteric effects of these compds. The thiophene ring could be replaced with benzene but not with several nitrogen-containing heterocycles. The 2-amino group was required, and at least one hydrogen on the amino group appeared to be necessary or activity. The keto carbonyl was also essential. Alkyl substitution at the 4-position of the thiophene ring increased activity, whereas 5-position substitution appeared to have little effect. Activity was also increased by various substitutions on the Ph ring, with 3-(trifluoromethyl) showing optimal activity. The Ph ring could be replaced with cyclohexyl without major loss of activity. 1-Aminofluoren-9-one, a conformationally locked derivative, was active. Based in part in the latter observation, the active conformation is proposed to have an intramol. hydrogen bond between the amino nitrogen and the carbonyl oxygen. Because the 2-amino-3-benzoylthiophenes showed competitive adenosine antagonism as well as allosteric enhancement, their affinities as competitive inhibitors of 8-[3H]cyclopentyl-1,3-dipropylxanthine binding to A1 receptors were also assessed. Structure-activity relations for competitive antagonism were distinct from those for allosteric enhancement, with ratios between the two activities varying by >1000-fold. Of the analogs tested, (2-amino-4,5-dimethyl-3-thienyl)-[3-(trifluoromethyl)phenyl]methanone (PD 81,723) had the most favorable ratio of enhancement to antagonism.

CC 1-3 (Pharmacology)

IT 82-45-1 91-02-1 117-99-7 119-61-9D, Benzophenone, derivs. 551-93-9  
 719-59-5 837-58-1 1016-78-0 1022-13-5 1137-41-3 1775-95-7



2835-77-0 2835-78-1 2894-51-1 4651-72-3 4651-96-1 4937-62-6  
5424-19-1 6344-62-3 6453-99-2 13129-17-4D, 4,5,6,7-  
Tetrahydrobenzo[b]thiophene, homologs 14548-46-0 21582-44-5  
21582-44-5D, 2-Amino-3-benzoylthiophene, derivs. 22283-10-9 24237-39-6  
24237-54-5 24248-69-9 24248-71-3 28059-64-5 29462-18-8, CI 718  
29462-25-7 29462-26-8 31272-19-2 36192-63-9 37023-77-1  
38009-49-3 40312-29-6 40312-30-9 40312-34-3 40312-51-4  
40487-75-0, PD 71605 42024-93-1 50508-69-5 50508-70-8 50798-30-6  
50838-03-4 52824-45-0 52824-46-1 52824-48-3 52824-61-0, PD 78416  
52824-68-7 52824-72-3 52824-77-8 52824-78-9 52824-81-4  
54493-47-9 54862-11-2 57226-72-9D, derivs. 57226-73-0 57226-74-1  
58192-84-0 68549-94-0 68751-90-6 69751-76-4 91411-44-8  
132861-87-1, PD 81723 132861-88-2, PD 117975 132897-83-7 132897-84-8  
132897-85-9 132897-86-0 132897-87-1 132897-88-2 132897-89-3  
132897-90-6 132897-91-7 132897-92-8 132897-93-9 132897-94-0  
132897-95-1 132897-96-2 132897-97-3 132897-98-4 132897-99-5  
132898-00-1 132898-01-2 132898-02-3 132915-40-3 132915-41-4  
132915-42-5 132942-77-9

RL: BIOL (Biological study)

(allosteric enhancement of adenosine A1 receptor binding by, structure  
in relation to)

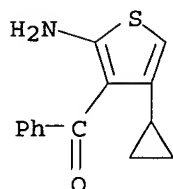
IT 68549-94-0

RL: BIOL (Biological study)

(allosteric enhancement of adenosine A1 receptor binding by, structure  
in relation to)

RN 68549-94-0 CAPLUS

CN Methanone, (2-amino-4-cyclopropyl-3-thienyl)phenyl- (9CI) (CA INDEX NAME)



L46 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:35597 CAPLUS

DOCUMENT NUMBER: 112:35597

TITLE: Synthesis and biological activity of substituted 2-  
and 3-cyclopropylthiophenes

AUTHOR(S): Surikova, T. P.; Zakharova, V. D.; Mochalov, S. S.;  
Shabarov, Yu. S.

CORPORATE SOURCE: II MMI im. Pirigova, MGU, Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1989), 23(7),  
840-3

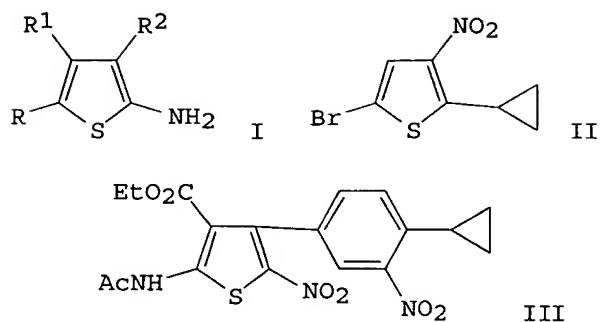
CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 112:35597

GI



AB Treating RCH<sub>2</sub>CR<sub>1</sub>:CR<sub>2</sub>CN (R = H, R<sub>1</sub> = cyclopropyl, R<sub>2</sub> = CO<sub>2</sub>Et, CONH<sub>2</sub>, cyano; R = H, Me, R<sub>1</sub> = p-cyclopropylphenyl, R<sub>2</sub> = CO<sub>2</sub>Et) with S in Et<sub>2</sub>NH gave 21-90% aminothiophenes I. Brominating 2-cyclopropylthiophene with NBS gave 90% 2-bromo-5-cyclopropylthiophene, which was nitrated by AcONO<sub>2</sub> to give 75% thiophene II. Acetylation of I (R = H, R<sub>1</sub> = cyclopropyl, R<sub>2</sub> = CO<sub>2</sub>Et) gave the N-acetyl derivative, which was nitrated by AcONO<sub>2</sub>-Ac<sub>2</sub>O to give 89% nitro(nitrophenyl)thiophene III. II was bactericidal against *Staphylococcus aureus* at a min. dose of 62.5 µg/mL.

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1

IT **29481-22-9P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and bromination of)

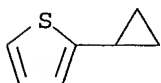
IT **120109-75-3P** 120109-76-4P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and sequential acetylation and nitration by acetyl nitrate)

IT 5424-47-5P 17407-30-6P 17407-32-8P 29481-26-3P **58124-28-0P**  
78113-02-7P 120109-72-0P 120109-73-1P 120109-74-2P  
**120109-77-5P** 120109-78-6P 120109-81-1P 120124-43-8P  
120124-44-9P 124557-47-7P 124557-48-8P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

IT **29481-22-9P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and bromination of)

RN 29481-22-9 CAPLUS

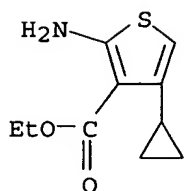
CN Thiophene, 2-cyclopropyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT **120109-75-3P**  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and sequential acetylation and nitration by acetyl nitrate)

RN 120109-75-3 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-4-cyclopropyl-, ethyl ester (9CI) (CA INDEX NAME)

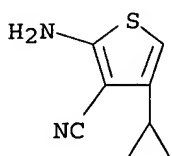


IT 58124-28-0P 120109-77-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

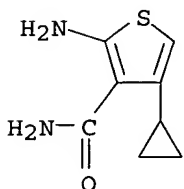
RN 58124-28-0 CAPLUS

CN 3-Thiophenecarbonitrile, 2-amino-4-cyclopropyl- (9CI) (CA INDEX NAME)



RN 120109-77-5 CAPLUS

CN 3-Thiophenecarboxamide, 2-amino-4-cyclopropyl- (9CI) (CA INDEX NAME)



L46 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:173025 CAPLUS

DOCUMENT NUMBER: 110:173025

TITLE: Synthesis and nitration of some 4-cyclopropyl- and 4-(p-cyclopropylphenyl)-2-aminothiophenes

AUTHOR(S): Surikova, T. P.; Zakharova, V. D.; Mochalov, S. S.; Shabarov, Yu. S.

CORPORATE SOURCE: Mosk. Gos. Univ., Moscow, 117234, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1988), (8), 1045-9

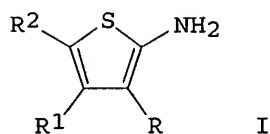
CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 110:173025

GI



AB Title thiophenes I (R = CO<sub>2</sub>Et, CONH<sub>2</sub>, CN; R<sub>1</sub> = cyclopropyl, p-cyclopropylphenyl; R<sub>2</sub> = H, Me) were prepared by cyclocondensation of crotononitriles R<sub>2</sub>CH<sub>2</sub>CR<sub>1</sub>:CRCN with sulfur in the presence Et<sub>2</sub>NH. Nitration of I with AcONO<sub>2</sub> at the thiophene C(2) position. With 10-fold excess agent, the benzene ring was nitrated at the m-position.

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

IT 17407-30-6P 17407-32-8P 58124-28-0P 120109-74-2P  
120109-77-5P  
RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(preparation of)

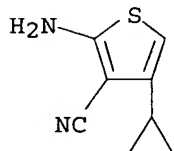
IT 120109-79-7P 120109-80-0P  
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**  
(preparation, nitration, and spectra of)

IT 120109-75-3P 120109-76-4P 120109-78-6P  
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**  
(preparation, N-acetylation, and spectra of)

IT 58124-28-0P 120109-77-5P  
RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(preparation of)

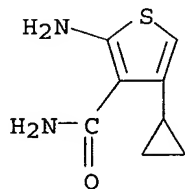
RN 58124-28-0 CAPLUS

CN 3-Thiophenecarbonitrile, 2-amino-4-cyclopropyl- (9CI) (CA INDEX NAME)



RN 120109-77-5 CAPLUS

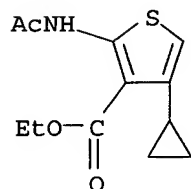
CN 3-Thiophenecarboxamide, 2-amino-4-cyclopropyl- (9CI) (CA INDEX NAME)



IT 120109-79-7P  
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**  
(preparation, nitration, and spectra of)

RN 120109-79-7 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-(acetylamino)-4-cyclopropyl-, ethyl ester  
(9CI) (CA INDEX NAME)

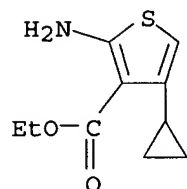


IT 120109-75-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation, N-acetylation, and spectra of)

RN 120109-75-3 CAPLUS

CN 3-Thiophenecarboxylic acid, 2-amino-4-cyclopropyl-, ethyl ester (9CI) (CA  
INDEX NAME)



L46 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1979:6430 CAPLUS

DOCUMENT NUMBER: 90:6430

TITLE: 6-Cyclopropyl-1,3-dihydro-1-methyl-5-phenyl-2-oxo-2H-  
thieno[2,3-e]diazepine

INVENTOR(S): Cognacq, Jean Claude

PATENT ASSIGNEE(S): Hexachimie S. A., Fr.

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

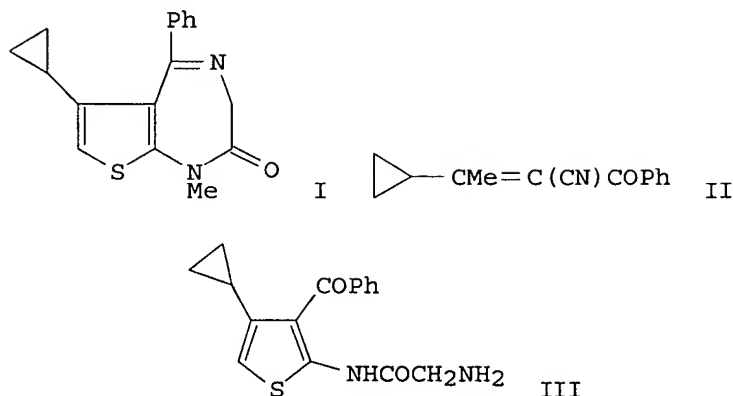
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2813996	A1	19781005	DE 1978-2813996	19780331
FR 2385721	A1	19781027	FR 1978-7697	19780316
ZA 7801694	A	19790328	ZA 1978-1694	19780323
BE 865278	A1	19780925	BE 1978-56799	19780324
JP 53121791	A2	19781024	JP 1978-35252	19780327
US 4156009	A	19790522	US 1978-890410	19780327
DK 7801354	A	19781001	DK 1978-1354	19780328
DD 137108	C	19790815	DD 1978-204460	19780329
DD 143777	C	19800910	DD 1978-213659	19780329
SE 7803604	A	19781001	SE 1978-3604	19780330
NO 7801102	A	19781003	NO 1978-1102	19780330
ES 468382	A1	19791001	ES 1978-468382	19780330

SU 715027	D	19800205	SU 1978-2594351	19780330
NL 7803431	A	19781003	NL 1978-3431	19780331
AU 7834956	A1	19791018	AU 1978-34956	19780411
ES 477164	A1	19791016	ES 1979-477164	19790125
PRIORITY APPLN. INFO.:			GB 1977-13587	A 19770331
GI				



AB The title compound (I) was prepared in 6 steps from PhCOCH<sub>2</sub>CN and cyclopropyl Me ketone via the cyclopropylcrotonitrile (II) and the aminoacetamidothiophene (III). The antiulcer activity of I was tabulated at various concns.

IC C07D495-04

CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))

IT **68549-95-1P**  
 RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)** (preparation and amination of)

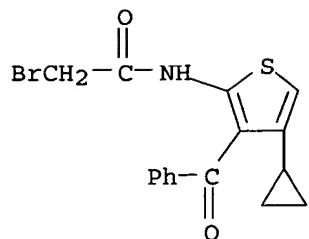
IT **68549-97-3P**  
 RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)** (preparation and methylation of)

IT **68549-94-0P**  
 RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)** (preparation and reaction with bromoacetyl bromide)

IT **68549-95-1P**  
 RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)** (preparation and amination of)

RN 68549-95-1 CAPLUS

CN Acetamide, N-(3-benzoyl-4-cyclopropyl-2-thienyl)-2-bromo- (9CI) (CA INDEX NAME)

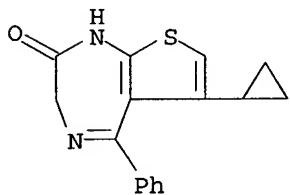


IT 68549-97-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and methylation of)

RN 68549-97-3 CAPLUS

CN 2H-Thieno[2,3-e]-1,4-diazepin-2-one, 6-cyclopropyl-1,3-dihydro-5-phenyl-  
(9CI) (CA INDEX NAME)

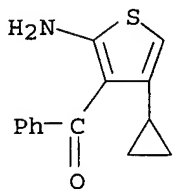


IT 68549-94-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(preparation and reaction with bromoacetyl bromide)

RN 68549-94-0 CAPLUS

CN Methanone, (2-amino-4-cyclopropyl-3-thienyl)phenyl- (9CI) (CA INDEX NAME)



L46 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:59172 CAPLUS

DOCUMENT NUMBER: 84:59172

TITLE: Thienyl ureas

INVENTOR(S): Kobzina, John W.

PATENT ASSIGNEE(S): Chevron Research Co., USA

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2510936	A1	19751009	DE 1975-2510936	19750313
US 3956315	A	19760511	US 1974-453231	19740321
CA 1040208	A1	19781010	CA 1975-220886	19750227
FR 2264814	A1	19751017	FR 1975-7935	19750313
FR 2264814	B1	19790608		
JP 50154427	A2	19751212	JP 1975-55557	19750320
GB 1462570	A	19770126	GB 1975-12037	19750321
			US 1974-453231	A 19740321

## PRIORITY APPLN. INFO.:

GI For diagram(s), see printed CA Issue.

AB Thienylureas I (R = CHMeEt, cyclopropyl, CMe<sub>3</sub>, CHMe<sub>2</sub>, Ph, cyclohexyl, R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Me; R = CMe<sub>3</sub>, CHMe<sub>2</sub>, cyclopropyl, R<sub>1</sub> = H, R<sub>2</sub> = R<sub>3</sub> = Me; R = CMe<sub>3</sub>, R<sub>1</sub> = Cl, R<sub>2</sub> = H, R<sub>3</sub> = Me; R = CMe<sub>3</sub>, CHMe<sub>2</sub>, CHMeEt, cyclopropyl, R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Pr, H, Et, CMe<sub>3</sub>) were prepared by treating the aminothiophenes with isocyanates. Thus, treatment of 2-amino-3-cyano-4-sec-butylthiophene with MeNCO gave I (R = CHMeEt, R<sub>1</sub> = R<sub>2</sub> = H, R<sub>3</sub> = Me), which at 5000 ppm post-emergent gave 80-100% control of weeds including wild oats and lambsquarters.

IC C07D; A01N

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 5

IT 10413-34-0 58124-26-8 **58124-28-0**

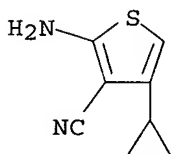
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with isocyanate)

IT **58124-28-0**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with isocyanate)

RN 58124-28-0 CAPLUS

CN 3-Thiophenecarbonitrile, 2-amino-4-cyclopropyl- (9CI) (CA INDEX NAME)





=> file casreact

FILE 'CASREACT' ENTERED AT 10:41:06 ON 22 MAR 2006  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 19 Mar 2006 VOL 144 ISS 12

New CAS Information Use Policies, enter HELP USAGETERMS for details.

\*\*\*\*\*  
\*  
\* CASREACT now has more than 10 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que nos L45

L14	STR
L16	947626 SEA FILE=REGISTRY ABB=ON PLU=ON SC4/ESS
L18	1954 SEA FILE=REGISTRY SUB=L16 SSS FUL L14
L33	STR
L35	2 SEA FILE=REGISTRY SUB=L18 SSS FUL L33
L45	0 SEA FILE=CASREACT ABB=ON PLU=ON L35/PRO

=> file caplus

FILE 'CAPLUS' ENTERED AT 10:41:26 ON 22 MAR 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Mar 2006 VOL 144 ISS 13  
FILE LAST UPDATED: 21 Mar 2006 (20060321/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d que nos L36

```
L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL L14
L33          STR
L35          2 SEA FILE=REGISTRY SUB=L18  SSS FUL L33
L36          2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L35
```

=> d que nos L41

```
L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL L14
L33          STR
L35          2 SEA FILE=REGISTRY SUB=L18  SSS FUL L33
L36          2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L35
L37          STR
L39          72 SEA FILE=REGISTRY SUB=L18  SSS FUL L37
L40          29 SEA FILE=CAPLUS ABB=ON  PLU=ON  L39
L41          1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L36 AND L40
```

=> d que nos L43

```
L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL L14
L33          STR
L35          2 SEA FILE=REGISTRY SUB=L18  SSS FUL L33
L43          2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L35/PREP
```

=> d que nos L44

```
L14          STR
L16          947626 SEA FILE=REGISTRY ABB=ON  PLU=ON  SC4/ESS
L18          1954 SEA FILE=REGISTRY SUB=L16  SSS FUL L14
L33          STR
L35          2 SEA FILE=REGISTRY SUB=L18  SSS FUL L33
L37          STR
L39          72 SEA FILE=REGISTRY SUB=L18  SSS FUL L37
L42          12 SEA FILE=CAPLUS ABB=ON  PLU=ON  L39 (L) (RGT OR RCT OR
             RACT)/RL
L43          2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L35/PREP
L44          1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L42 AND L43
```

=> s L36 or L41 or L43 or L44

```
L47          2 L36 OR L41 OR L43 OR L44
```

=> d ibib abs hitind hitstr L47 1-2

L47 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:390242 CAPLUS

DOCUMENT NUMBER: 140:406731

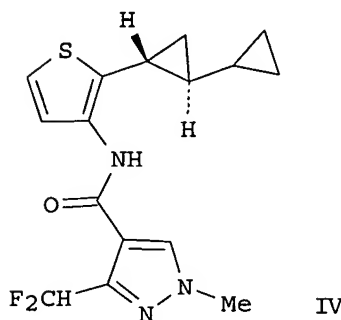
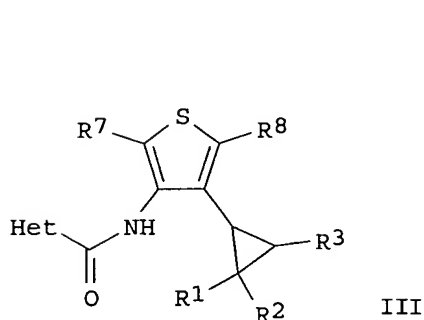
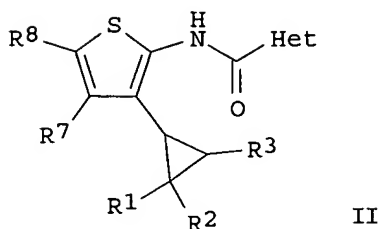
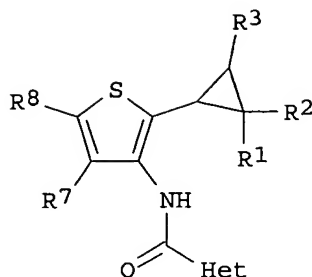
TITLE: Preparation of N-(cyclopropylthienyl)carboxamides as fungicides

INVENTOR(S): Ehrenfreund, Josef; Tobler, Hans; Walter, Harald

PATENT ASSIGNEE(S): Syngenta Participations Ag, Switz.

SOURCE: PCT Int. Appl., 43 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039799	A1	20040513	WO 2003-EP11805	20031024
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2501739	AA	20040513	CA 2003-2501739	20031024
AU 2003286140	A1	20040525	AU 2003-286140	20031024
EP 1556377	A1	20050727	EP 2003-776869	20031024
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003015857	A	20050920	BR 2003-15857	20031024
JP 2006508089	T2	20060309	JP 2004-547558	20031024
US 2006030567	A1	20060209	US 2005-532847	20050427
PRIORITY APPLN. INFO.:			GB 2002-25554	A 20021101
			WO 2003-EP11805	W 20031024
OTHER SOURCE(S):	MARPAT 140:406731			
GI				



AB A fungicidally active compound I, II, or III [wherein Het = (un)substituted 5- or 6-membered heterocyclic ring containing one to three O, N, and/or S atoms, provided that the ring is not 1,2,3-triazole; R1 and R2 = independently H, halo, or Me; R3 = (un)substituted (cyclo)alkyl, alkenyl, alkynyl, Ph, heterocyclyl; R7 and R8 = independently H, halo, or (halo)alkyl] were prepared for use as active ingredients in agricultural or horticultural compns. for controlling or preventing infestation of plants by phytopathogenic microorganisms, preferably fungi. For example, 3-difluoromethyl-1-methyl-1H-pyrazole-4-carboxylic acid was amidated with [2-(bicyclopropyl-2-yl)thiophen-3-yl]amine in the presence of TEA and N,N-bis(2-oxooxazolidinyl)phosphinic acid chloride in CH<sub>2</sub>Cl<sub>2</sub> to give trans-IV (97% purity). The latter showed excellent activity against *Puccinia recondita* on wheat (0-5% infestation) and showed good activity against *Podosphaera leucotricha* on apple, *Venturia inaequalis* on apple, *Erysiphe graminis* on barley, *Pyrenophora teres* on barley, *Alternaria solani* on tomato, and *Uncinula necator* on grape (<20% infestation for each).

IC ICM C07D409-12

ICS C07D411-12; C07D417-12; C07D333-36; A01N043-56; A01N043-36; A01N043-78; A01N043-40; A01N043-32

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 10

IT 688328-34-9P, (2E)-3-(3-Bromothiophen-2-yl)-1-cyclopropylprop-2-en-1-one  
688328-35-0P 688328-36-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(intermediate; preparation of N-(cyclopropylthienyl)carboxamides as fungicides)

IT 688328-35-0P 688328-36-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

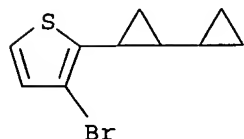
(Preparation); RACT (Reactant or reagent)

(intermediate; preparation of N-(cyclopropylthienyl)carboxamides as

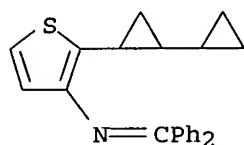
fungicides)

RN 688328-35-0 CAPLUS

CN Thiophene, 2-[1,1'-bicyclopropyl]-2-yl-3-bromo- (9CI) (CA INDEX NAME)



RN 688328-36-1 CAPLUS

CN 3-Thiophenamine, 2-[1,1'-bicyclopropyl]-2-yl-N-(diphenylmethylene)- (9CI)  
(CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:202482 CAPLUS

DOCUMENT NUMBER: 138:238189

TITLE: Preparation of thienooxazin-4-ones as lipase  
inhibitors for treatment of obesity and related  
disorders

INVENTOR(S): Hodson, Harold Francis; Dunk, Christopher Robert;  
Palmer, Richard Michael John; Mitchell, Dale Robert;  
Birault, Veronique; Hunt, Russell George

PATENT ASSIGNEE(S): Alizyme Therapeutics Limited, UK

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

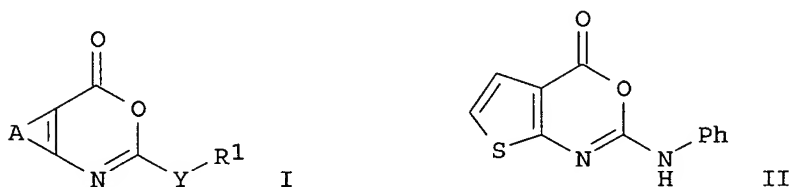
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003020282	A1	20030313	WO 2002-GB3903	20020823
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2458213	AA	20030313	CA 2002-2458213	20020823
EP 1446125	A1	20040818	EP 2002-755241	20020823

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

CN 1556706	A	20041222	CN 2002-818590	20020823
JP 2005527469	T2	20050915	JP 2003-524589	20020823
ZA 2004001595	A	20050225	ZA 2004-1595	20040225
NO 2004001295	A	20040329	NO 2004-1295	20040329
US 2005075336	A1	20050407	US 2004-488045	20041101
PRIORITY APPLN. INFO.:			GB 2001-21019	A 20010830
			GB 2002-6031	A 20020314
			WO 2002-GB3903	W 20020823

OTHER SOURCE(S): MARPAT 138:238189

GI



AB Title compds. I [wherein A = (un)substituted thienyl moiety; Y = O, S, or NR<sub>2</sub>; R<sub>1</sub> = (un)substituted alkyl optionally interrupted by one or more O atoms, (cyclo)alkenyl, alkynyl, cycloalkyl, (hetero)aryl, (hetero)arylalkyl, reduced (hetero)arylalkyl, (hetero)arylalkenyl, or reduced (hetero)aryl; R<sub>2</sub> = H or a group as defined for R<sub>1</sub>; or salts, esters, amides, or prodrugs thereof] were prepared as lipase inhibitors. For example, reaction of tert-Bu 2-aminothiophene-3-carboxylate with Ph isocyanate provided tert-Bu 2-(phenylureido)-3-thiophenecarboxylate, which was treated with TFA to give the acid. Cyclization using EDC afforded 2-phenylamino-4H-thieno[2,3-d][1,3]oxazin-4-one (II). The latter inhibited human pancreatic lipase and porcine pancreatic lipase with IC<sub>50</sub> values of < 100 nM and ≤ 1 μM, resp. Thus, I are useful for the treatment of obesity and related disorders, such as hyperlipemia, hyperlipidemia, hyperglycemia, hypertension, cardiovascular disease, or a stroke gastrointestinal disease or condition (no data). In addition, I may be used in preventing the degradation of foodstuff which comprises a fat and in the manufacture of surfactants, soaps, or detergents.

IC ICM A61K031-535

ICS C07D498-04; C07D498-16

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 17, 62

IT 109666-64-0P, 5,6-Dimethyl-2-phenylamino-4H-thieno[2,3-d][1,3]oxazin-4-one  
109666-70-8P, 2-Phenylamino-4H-thieno[2,3-d][1,3]oxazin-4-one  
111423-21-3P, 2-Phenylamino-5,6,7,8-tetrahydro-4H-benzothieno[2,3-d][1,3]oxazin-4-one 501366-53-6P, 2-[(4-Phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-59-2P, 2-[(4-Phenylsulfanylphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
501366-63-8P, 6-Methyl-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-66-1P, 6-Methyl-2-phenylamino-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-67-2P, 2-Butylamino-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-68-3P, 2-Butyloxy-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-69-4P, 5-Methyl-2-phenylamino-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-70-7P, 6-Phenyl-2-phenylamino-4H-thieno[3,2-d][1,3]oxazin-4-one 501366-71-8P, 2-[[4-(3-Trifluoromethylphenoxy)phenyl]amino]-4H-

thieno[2,3-d][1,3]oxazin-4-one 501366-72-9P, 6-(1,1-Dimethylethyl)-2-phenylamino-4H-thieno[3,2-d][1,3]oxazin-4-one 501366-73-0P, 2-[(4-Phenoxyphenyl)amino]-4H-thieno[3,2-d][1,3]oxazin-4-one 501366-74-1P, 2-[(4-Phenylmethylphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-75-2P, 2-[(4-Benzoylphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-76-3P, 6-Methyl-2-(4-phenoxyphenoxy)-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-77-4P, 2-[[4-(4-Trifluoromethylphenoxy)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-78-5P, 2-[4-(3-Trifluoromethylphenoxy)phenoxy]-4H-thieno[3,2-d][1,3]oxazin-4-one 501366-79-6P, 5,6-Dimethyl-2-(4-phenoxyphenoxy)-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-80-9P, 2-Dodecylamino-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-81-0P, 2-(N-Dodecyl-N-methylamino)-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-82-1P, 2-Dodecylamino-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-83-2P, 2-Dodecylthio-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-84-3P, 2-[[4-[N-(1-Methylethyl)-N-phenylamino]phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-85-4P, 2-[[4-(Phenylsulfonyl)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-86-5P, 2-[[4-(Phenylcarbamoyl)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-87-6P, 2-[[4-(4-Chlorophenoxy)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-88-7P, 2-[[4-(4-Methylphenoxy)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-89-8P, 2-[(4-Cyanophenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-90-1P, 2-[(4-Cyanophenyl)amino]-6-propyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-91-2P, 2-[(4-Cyanophenyl)amino]-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-92-3P, 6-Phenylmethyl-2-[(4-cyanophenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-93-4P, 2-[(4-Cyanophenyl)amino]-6-dodecyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-94-5P, 6-Methyl-2-[(4-phenylbutyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-95-6P, 2-[(2-Chloroethyl)amino]-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-96-7P, 2-[(Hept-6-enyl)amino]-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-97-8P, 2-[(5-Methoxycarbonylpentyl)amino]-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501366-98-9P, 2-[(4-Phenoxyphenyl)amino]-4H-thieno[3,4-d][1,3]oxazin-4-one 501366-99-0P, 2-[[4-(4-Trifluoromethylphenoxy)phenyl]amino]-4H-thieno[3,2-d][1,3]oxazin-4-one 501367-00-6P, 2-[(4-Cyanophenyl)amino]-4H-thieno[3,2-d][1,3]oxazin-4-one 501367-01-7P, 2-Dodecylamino-4H-thieno[3,2-d][1,3]oxazin-4-one 501367-02-8P, 2-[(5-Methylhexyl)amino]-4H-thieno[3,2-d][1,3]oxazin-4-one 501367-03-9P, 6-Methyl-2-[(4-phenoxyphenyl)amino]-4H-thieno[3,2-d][1,3]oxazin-4-one 501367-04-0P, 6-Propyl-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-05-1P, 2-Hexadecylamino-6-methyl-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-06-2P, 6-Chloro-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-07-3P, 6-Dodecyl-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-08-4P, 6-Phenylmethyl-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-09-5P, 501367-10-8P, 2-[(5,5,5-Trifluoropentyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-11-9P, 2-Eicosylamino-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-12-0P, 2-Octadecylamino-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-13-1P, 2-Hexadecyloxy-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-14-2P, 2-[(12-Nitrododecyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-15-3P, 2-[(12-Phenyldodecyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-16-4P, 2-[[12-(Pyrid-2-yl)dodecyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-17-5P, 2-Octylamino-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-18-6P, 2-[(8-Phenylloctyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-19-7P, 2-[(4-Phenylsulfinylphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-20-0P, 2-[(4-Phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-21-1P, 2-[[4-(4-Methoxyphenoxy)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-22-2P, 2-[[4-(4-Dimethylaminophenoxy)phenyl]a

mino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-23-3P,  
 2-[[4-(4-Hydroxyphenoxy)phenyl]amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-24-4P, 2-[(3-Phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-25-5P, 2-[(2-Phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-26-6P, 2-[(3-Cyanophenyl)amino]-6-methyl-4H-thieno[2,3-  
 d][1,3]oxazin-4-one 501367-27-7P, 2-[(4-Chlorophenyl)amino]-6-methyl-4H-  
 thieno[2,3-d][1,3]oxazin-4-one 501367-28-8P, 2-[(4-Aminophenyl)amino]-4H-  
 thieno[2,3-d][1,3]oxazin-4-one 501367-29-9P, 2-[(4-Hydroxyphenyl)amino]-  
 4H-thieno[2,3-d][1,3]oxazin-4-one 501367-30-2P, 2-[(4-  
 Methoxycarbonylphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-31-3P, 2-[(4-Trifluoromethylphenyl)amino]-4H-thieno[2,3-  
 d][1,3]oxazin-4-one 501367-32-4P, 2-[N-(4-Phenoxyphenyl)-N-ethylamino]-  
 4H-thieno[2,3-d][1,3]oxazin-4-one 501367-33-5P, 2-[N-(4-Phenoxyphenyl)-N-  
 (1-methylethyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-34-6P, 6-Cyclopropyl-2-[(4-phenoxyphenyl)amino]-4H-  
 thieno[2,3-d][1,3]oxazin-4-one 501367-35-7P, 2-[(4-Phenoxyphenyl)thio]-  
 4H-thieno[2,3-d][1,3]oxazin-4-one 501367-36-8P, 2-[(4-  
 Phenoxyphenyl)amino]-6-trifluoromethyl-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-37-9P, 6-Methoxy-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-  
 d][1,3]oxazin-4-one 501367-38-0P, 6-Phenoxy-2-[(4-phenoxyphenyl)amino]-  
 4H-thieno[2,3-d][1,3]oxazin-4-one 501367-39-1P, 6-Methyl-2-[(4-  
 methoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one 501367-40-4P,  
 6-Cyano-2-[(4-phenoxyphenyl)amino]-4H-thieno[2,3-d][1,3]oxazin-4-one  
 501367-41-5P, 6-Methyl-2-[(4-phenoxyphenyl)thio]-4H-thieno[2,3-  
 d][1,3]oxazin-4-one 501367-42-6P, 6-Methyl-2-(4-phenoxyphenoxy)-4H-  
 thieno[3,2-d][1,3]oxazin-4-one 501367-43-7P, 7-Methyl-2-[(4-  
 phenoxyphenyl)amino]-4H-thieno[3,4-d][1,3]oxazin-4-one 501367-44-8P,  
 5-Methyl-2-[(4-phenoxyphenyl)amino]-4H-thieno[3,4-d][1,3]oxazin-4-one  
 501367-45-9P, 6-Methyl-2-[(3-methylisoxazol-5-yl)amino]-4H-thieno[2,3-  
 d][1,3]oxazin-4-one

RL: COS (Cosmetic use); FFD (Food or feed use); MOA (Modifier or additive  
 use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation);  
 USES (Uses)

(lipase inhibitor; preparation of thienooxazinones as lipase inhibitors for  
 treatment of obesity and related disorders)

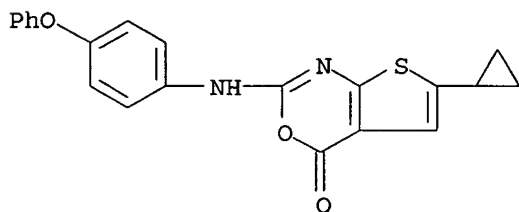
IT 501367-34-6P, 6-Cyclopropyl-2-[(4-phenoxyphenyl)amino]-4H-  
 thieno[2,3-d][1,3]oxazin-4-one

RL: COS (Cosmetic use); FFD (Food or feed use); MOA (Modifier or additive  
 use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation);  
 USES (Uses)

(lipase inhibitor; preparation of thienooxazinones as lipase inhibitors for  
 treatment of obesity and related disorders)

RN 501367-34-6 CAPLUS

CN 4H-Thieno[2,3-d][1,3]oxazin-4-one, 6-cyclopropyl-2-[(4-  
 phenoxyphenyl)amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS



Qazi 10/532847

03/22/2006

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

**THIS PAGE BLANK (USPTO)**